Supporting Information

Synthesis of spirotriazolines and spirooxadiazolines *via* light-induced 1,3-dipolar [3 + 2] cycloadditions

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1. General information

Unless noted, all reactions were carried out in flame-dried glassware with magnetic stirring under an atmosphere of air. Chemicals and solvents were either purchased from commercial suppliers or purified by standard techniques. All the reactions were monitored by thin-layer chromatography (TLC) and were visualized using UV light. The product purification was done using silica gel column chromatography. Thin-layer chromatography (TLC) characterization was performed with precoated silica gel GF254 (0.2mm), while column chromatography characterization was performed with silica gel (100-200 mesh). NMR spectra were recorded on a Varian spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C and 376 MHz for ^{19}F). Chemical shifts are reported in δ ppm referenced to an internal $SiMe_4$ standard for ^{1}H NMR and chloroform-*d* (δ 77.16) for ^{13}C NMR. Coupling constants were given in Hz. The photoreactor used in this research was the Ultraviolet high-pressure Hg lamp bought from Shanghai Bilang Instrument Co., Ltd. HRMS spectra were recorded on a Waters Q-TOF Premier. Melting points were measured with YRT-3 melting point apparatus (Shantou Keyi Instrument & Equipment Co., Ltd., Shantou, China).

Pyrazolon-derived phenyl-ketimine **2a-2d**[1], N-aryl substituted isoquinolinone, isoquinoline-1,3,4(2*H*)-triones **4a**[2, 3] were prepared according to the literature.

2. Experimental procedures

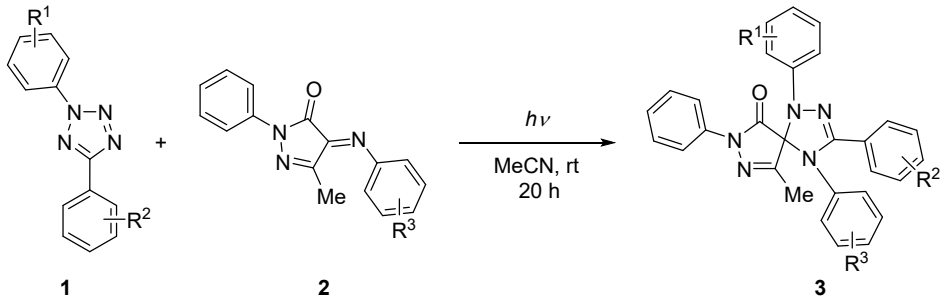
2.1 General Procedure A: Synthesis of 2,5-diaryltetrazoles 1a-1e and 1g-1l[4]

A solution of 5-phenyltetrazole (1 equiv.), aryl boronic acid (2 equiv.), and copper(I) oxide (0.05 equiv.) in DMSO (2 mL/mmol) was stirred under an O2 atmosphere at 110 ºC until full consumption of the starting material was observed. The reaction mixture was cooled, diluted with DCM, and washed successively with 1M HCl and brine. The solution was passed through a phase separator, concentrated under vacuum and purified by column chromatography.

2.2 General Procedure B: Synthesis of 2,5-diaryltetrazoles 1f and 1m-1t[5,6]

Aldehyde (1 equiv.) was added to a solution of phenylsulfonylhydrazide (1 equiv.) in absolute ethanol (1.0 M). After stirring for 1 h at room temperature the mixture was diluted with water resulting in the precipitation of sulfonylhydrazone. The precipitate was collected by filtration, washed with aqueous ethanol and dried under vacuum and was used in the subsequent transformation without further purification. Simultaneously, a solution of $NaNO_2$ (1 equiv.) in H_2O (2.5 M) was slowly added to a solution of aniline (1 g, 1 equiv.) in a 50% mixture of EtOH and H_2O (0.62 M) and concentrated HCl (1.3 mL/5 mmol of aniline) at 0 ºC. After 30 min, this solution was carefully added to a solution of the corresponding benzensufonohydrazone (1 equiv.) in pyridine (0.16 M) at -15 ºC. Once the addition is completed, the mixture was allowed to warm at rt during 1 h. After this time, HCl (10%) was added, and the resulting mixture was extracted with $CHCl_3$ (x3). The combined organic layers were dried over Na_2SO_4 and concentrated under vacuum. The residue was purified by flash chromatography.

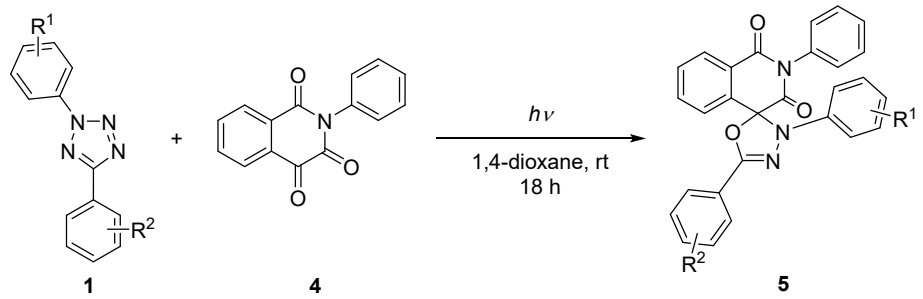
2.3 General Procedure C: Light-Induce 1,3-dipolar reaction between pyrazolon-derived phenyl-ketimine and 2,5-diaryltetrazoles



1 **2** **3**

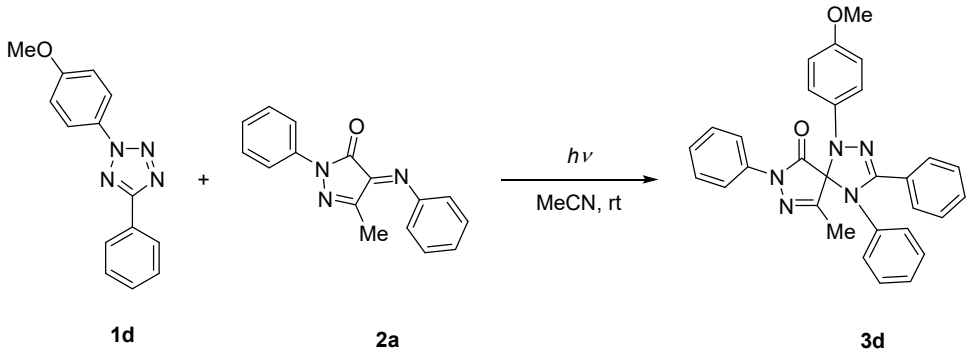
A quartz vessel containing a solution of pyrazolon-derived phenyl-ketimine **2** (0.10 mmol, 1 equiv.) and the corresponding 2,5-diaryltetrazole **1** (0.15 mmol, 1.5 equiv.) in MeCN (2 mL) was irradiated with an Ultraviolet high-pressure Hg lamp for 20 h. MeCN was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, PE/EtOAc = 8/1) to give the corresponding compound **3**.

2.4 General Procedure D: Light-Induce 1,3-dipolar reaction between isoquinoline-1,3,4(2*H*)-triones and 2,5-diaryltetrazoles



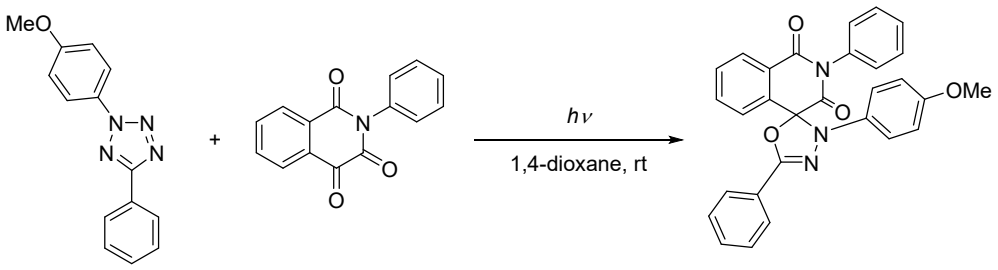
A quartz vessel containing a solution of isoquinoline-1,3,4(2*H*)-triones **4** (0.10 mmol, 1 equiv.) and the corresponding 2,5-diaryltetrazole **1** (0.15 mmol, 1.5 equiv.) in 1,4-dioxane (2 mL) was irradiated with an Ultraviolet high-pressure Hg lamp for 18 h. 1,4-dioxane was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, PE/EtOAc = 6/1) to give the corresponding compound **5**.

2.5 Gram-scale synthesis of spirotriazoline 3d



A round-bottom flask containing a solution of pyrazolon-derived phenyl-ketimine **2a** (1 g, 3.8 mmol, 1 equiv.) and the corresponding 2,5-diaryltetrazole **1d** (1.44g, 5.7 mmol, 1.5 equiv.) in MeCN (25 mL) was irradiated with an Ultraviolet high-pressure Hg lamp. After the reaction completed (monitored by TLC), MeCN was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, PE/EtOAc = 8/1) to give the corresponding compound **3d** as yellow solid in 88% yield (1.53 g).

2.6 Gram-scale synthesis of spirooxadiazoline 5d



1d **4a** **5d**

A round-bottom flask containing a solution of isoquinoline-1,3,4(2*H*)-triones **4a** (1 g, 3.98 mmol, 1 equiv.) and the corresponding 2,5-diaryltetrazole **1d** (1.51 g, 5.97 mmol, 1.5 equiv.) in 1,4-dioxane (25 mL) was irradiated with an Ultraviolet high-pressure Hg lamp. After the reaction completed (monitored by TLC), 1,4-dioxane was removed under reduced pressure, and the residue was purified by column chromatography (silica gel, PE/EtOAc = 6/1) to give the corresponding compound **5d** as yellow solid in 92% yield (1.63 g).

3. Detecting the reaction by ^{1}H NMR

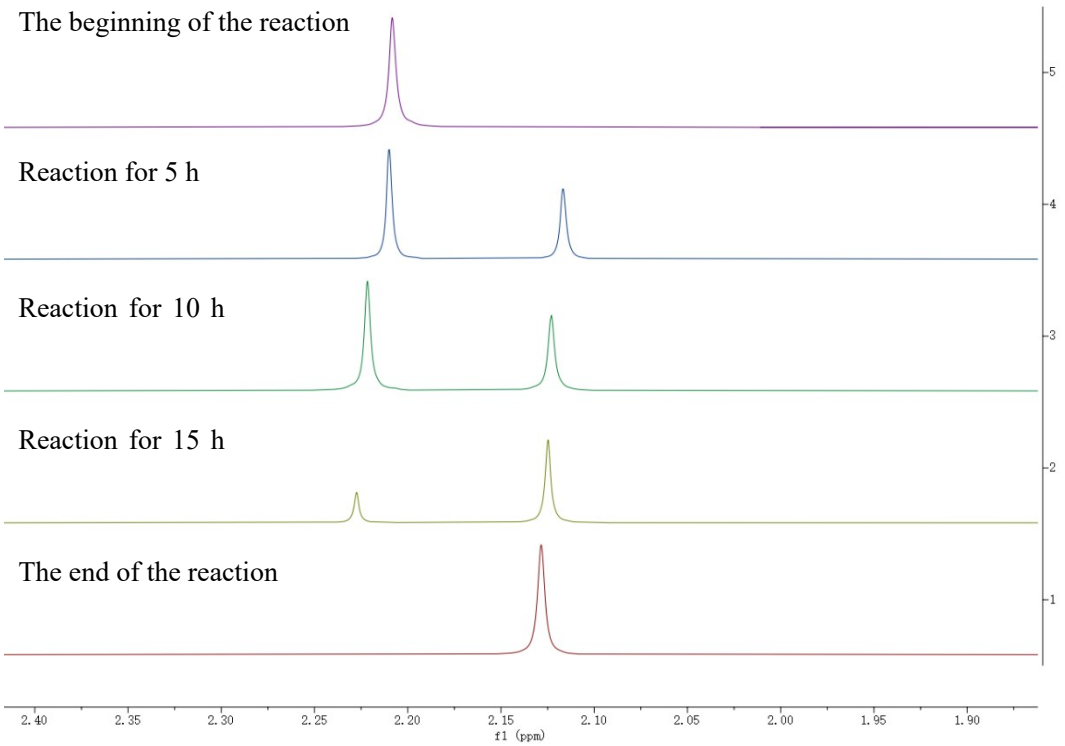


Figure S1. Detecting the reaction by ^{1}H NMR

Five quartz vessels containing a solution of pyrazolon-derived phenyl-ketimine **2a**

(26.3 mg, 0.10 mmol, 1 equiv.) and the corresponding 2,5-diaryltetrazole **1a** (33.3 mg, 0.15 mmol, 1.5 equiv.) in MeCN (2 mL) was irradiated with an Ultraviolet high-pressure Hg lamp for 5 h, 10h, 15h, 20h. MeCN was removed under reduced pressure, and the residue was detected by ^{1}H NMR.

4. Irradiation lamps details

Figure S2. Reaction set-up. Ultraviolet high-pressure Hg lamp as UV-light irradiation (UV λ = 365 nm)

5 References

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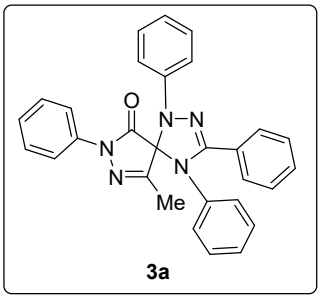
6 Ortiz-Rojano, L.; Rojas-Martin, J.; Rodriguez-Diaz, C.; Carreno, M. C.; Ribagorda, M., *Chemistry* **2019,** *25*, 15050-15054.

6. Characterization data of all compounds

6.1 Characterization data of spirotriazolines

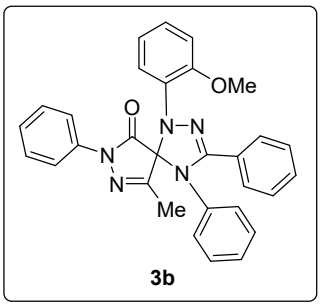
9-methyl-1,3,4,7-tetraphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3a)



3a

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1a** (33.3 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3a** as yellow solid after flash column chromatography (44.4 mg, 97% yield). M.p.: 238-239 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 (d, *J* = 8.1 Hz, 2H), 7.55 – 7.44 (m, 2H), 7.33 (dt, *J* = 14.1, 7.5 Hz, 3H), 7.29 – 7.23 (m, 3H), 7.18 (tt, *J* = 11.6, 6.4 Hz, 5H), 6.99 (t, *J* = 7.8 Hz, 4H), 6.88 (t, *J* = 7.3 Hz, 1H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.54, 158.06, 148.16, 142.82, 137.40, 137.36, 129.78, 129.55, 129.46, 129.02, 128.38, 128.05, 127.49, 126.72, 126.60, 125.80, 121.16, 119.02, 113.86, 89.18, 13.87. HRMS calcd for $C_{29}H_{23}N_5NaO$ $[M+Na]^+$: 480.1800, found for: 480.1801

1-(2-methoxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3b)

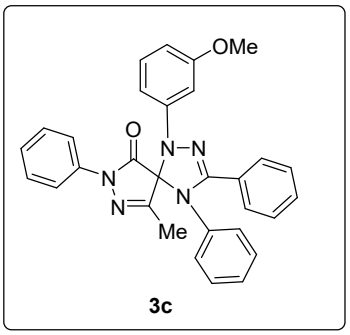


3b

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1b** (37.8 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3b** as yellow solid after flash column chromatography (47.3 mg, 97% yield). M.p.: 225-227 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.65 (m, 2H), 7.52 – 7.47 (m, 2H), 7.39 – 7.29 (m, 3H), 7.29 – 7.22 (m, 3H), 7.17 (qd, *J* = 8.6, 7.6, 4.1 Hz, 4H), 7.08 (t, *J* = 8.2 Hz, 1H), 7.00 – 6.95 (m, 2H), 6.70 (t, *J* = 2.3 Hz, 1H), 6.45 (ddd, *J* = 8.5, 6.3, 2.3 Hz, 2H), 3.69 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.55, 160.83, 158.08, 148.09, 143.95, 137.38, 137.29, 130.35, 129.80, 129.46, 129.01, 128.37, 128.07, 127.54, 126.66, 125.80, 118.97, 107.28, 105.59, 99.54, 89.05, 55.16,

13.85. HRMS calcd for $C_{30}H_{25}N_5NaO_2$ $[M+Na]^+$: 510.1906, found for: 510.1907.

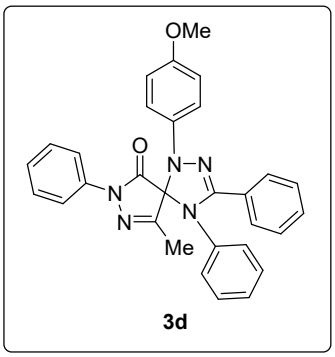
1-(3-methoxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3c)



3c

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1c** (37.8 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3c** as yellow solid after flash column chromatography (46.8 mg, 96% yield). M.p.: 246-247 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (dd, *J* = 20.7, 7.6 Hz, 3H), 7.55 – 7.47 (m, 2H), 7.35 – 7.28 (m, 3H), 7.27 – 7.22 (m, 2H), 7.13 (dt, *J* = 9.9, 6.4 Hz, 4H), 7.03 – 6.92 (m, 4H), 6.73 (dd, *J* = 7.3, 2.1 Hz, 1H), 3.44 (s, 3H), 2.06 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.46, 158.11, 149.76, 149.62, 137.93, 137.57, 134.31, 129.73, 129.23, 128.87, 128.30, 128.24, 127.38, 127.01, 126.96, 124.91, 124.04, 121.50, 121.25, 118.27, 110.56, 90.23, 54.39, 14.14. HRMS calcd for $C_{30}H_{25}N_5NaO_2$ $[M+Na]^+$: 510.1906, found for: 510.1905.

1-(4-methoxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3d)

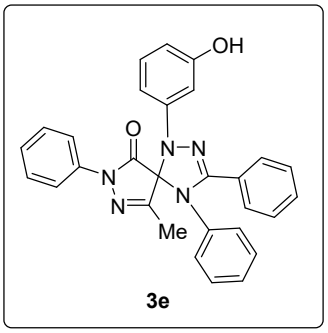


3d

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1d** (37.8 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3d** as yellow solid after flash column chromatography (43.9 mg, 90% yield). M.p.: 202-203 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.53 – 7.46 (m, 2H), 7.37 – 7.29 (m, 3H), 7.26 (dd, *J* = 8.4, 6.5 Hz, 2H), 7.15 (dt, *J* = 14.6, 7.3 Hz, 4H), 7.00 (d, *J* = 8.6 Hz, 2H), 6.95 (dd, *J* = 7.5, 1.9 Hz, 2H), 6.81 – 6.74 (m, 2H), 3.71 (s, 3H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.43, 158.34, 155.02, 148.17, 137.62, 137.42, 137.15, 129.67, 129.40, 128.97, 128.35, 128.00, 127.15, 126.86, 126.19, 125.69, 118.96, 116.90, 114.77, 90.19, 55.50, 13.98. HRMS calcd for

$C_{30}H_{26}N_5O_2$ $[M+H]^+$: 488.2087, found for: 488.2088.

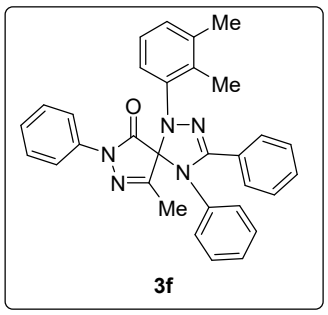
1-(3-hydroxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3e)



3e

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1e** (35.7 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3e** as yellow solid after flash column chromatography (45.9 mg, 97% yield). M.p.: 243-244 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (d, *J* = 8.0 Hz, 2H), 7.50 – 7.42 (m, 2H), 7.32 (dt, *J* = 14.8, 7.4 Hz, 3H), 7.28 – 7.20 (m, 3H), 7.16 (p, *J* = 6.9, 6.3 Hz, 4H), 7.01 – 6.93 (m, 3H), 6.74 (t, *J* = 2.3 Hz, 1H), 6.30 (ddd, *J* = 19.2, 8.1, 2.3 Hz, 2H), 2.22 (s, 3H), 1.26 (s, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.68, 158.33, 157.09, 148.30, 143.97, 137.25, 137.18, 130.54, 129.83, 129.47, 129.04, 128.38, 128.09, 127.58, 126.67, 126.53, 125.94, 119.19, 108.63, 105.18, 101.97, 89.20, 13.83. HRMS calcd for $C_{29}H_{23}N_5NaO_2$ $[M+Na]^+$: 496.1749, found for: 496.1748.

1-(2,3-dimethylphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3f)

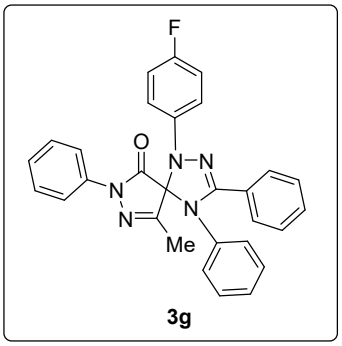


3f

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1f** (37.5 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3f** as yellow solid after flash column chromatography (47.1 mg, 97% yield). M.p.: 260-261 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (dd, *J* = 13.0, 7.8 Hz, 4H), 7.30 (td, *J* = 9.3, 7.3, 4.3 Hz, 6H), 7.19 – 7.02 (m, 5H), 6.97 (d, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 7.6 Hz, 2H), 2.19 (d, *J* = 7.7 Hz, 6H), 2.12 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.42, 157.71, 149.79, 142.57, 138.15, 138.07, 137.39, 132.38, 129.73, 129.34, 128.90, 128.36, 128.09, 128.00, 127.03, 126.68, 125.79, 125.51, 125.47, 123.96, 118.88, 91.18, 20.62, 15.10, 14.64. HRMS calcd for $C_{31}H_{28}N_5O$ $[M+H]^+$: 486.2294,

found for: 486.2293.

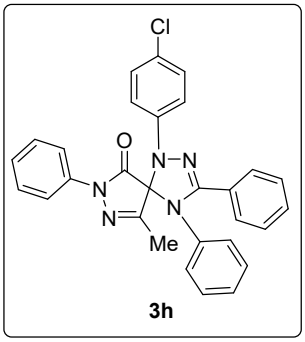
1-(4-fluorophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3g)



3g

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1g** (36.0 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3g** as yellow solid after flash column chromatography (41.5 mg, 88% yield). M.p.: 248-249 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.63 (m, 2H), 7.51 – 7.45 (m, 2H), 7.38 – 7.30 (m, 3H), 7.29 – 7.22 (m, 2H), 7.22 – 7.11 (m, 4H), 7.02 – 6.89 (m, 6H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.35, 159.24, 158.04, 156.85, 148.58, 139.52 (d, *J* = 2.4 Hz), 137.30 (d, *J* = 4.3 Hz), 129.89, 129.49, 129.04, 128.41, 128.06, 127.46, 126.59, 126.41, 125.87, 118.94, 116.10 (d, *J* = 30.7 Hz), 116.03, 89.68, 13.90. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -122.31. HRMS calcd for $C_{29}H_{22}FN_5NaO$ $[M+Na]^+$: 498.1706, found for: 498.1705.

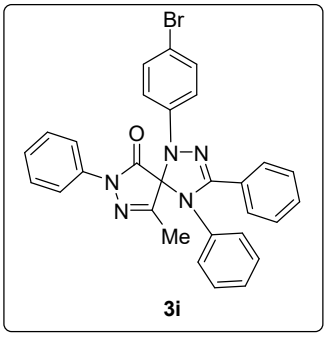
1-(4-chlorophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3h)



3h

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1h** (38.5 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3h** as yellow solid after flash column chromatography (44.2 mg, 90% yield). M.p.: 239-240 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 – 7.64 (m, 2H), 7.48 (dt, *J* = 7.0, 1.5 Hz, 2H), 7.40 – 7.30 (m, 3H), 7.29 – 7.23 (m, 2H), 7.22 – 7.12 (m, 6H), 7.00 – 6.95 (m, 2H), 6.94 – 6.90 (m, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.20, 157.77, 148.61, 141.44, 137.23, 137.12, 129.98, 129.53, 129.48, 129.07, 128.43, 128.08, 127.65, 126.59, 126.43, 125.95, 118.95, 114.99, 89.03, 13.85. HRMS calcd for $C_{29}H_{22}ClN_5NaO$ $[M+Na]^+$: 514.1411, found for: 514.1410.

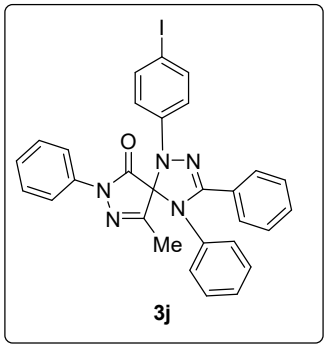
1-(4-bromophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3i)



3i

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1i** (45.2 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3i** as yellow solid after flash column chromatography (49.7 mg, 93% yield). M.p.: 269-271 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.64 (m, 2H), 7.52 – 7.46 (m, 2H), 7.39 – 7.27 (m, 6H), 7.24 (d, *J* = 1.7 Hz, 1H), 7.23 – 7.12 (m, 4H), 7.00 – 6.94 (m, 2H), 6.89 – 6.84 (m, 2H), 2.22 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.17, 157.71, 148.62, 141.82, 137.22, 137.08, 132.37, 130.00, 129.54, 129.08, 128.44, 128.09, 127.69, 126.62, 126.41, 125.96, 118.96, 115.28, 113.25, 88.91, 13.85. HRMS calcd for $C_{29}H_{22}BrN_5NaO$ $[M+Na]^+$: 558.0905, found for: 558.0906.

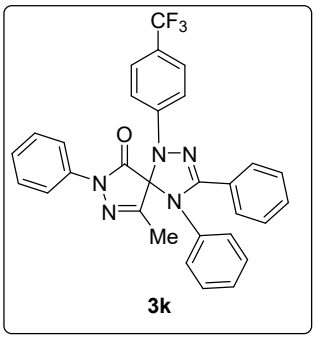
1-(4-iodophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3j)



3j

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1j** (52.2 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3j** as yellow solid after flash column chromatography (56.0 mg, 96% yield). M.p.: 236-237 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.56 (m, 2H), 7.43 – 7.37 (m, 4H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.25 – 7.22 (m, 1H), 7.21 – 7.15 (m, 3H), 7.10 (td, *J* = 9.3, 6.8 Hz, 4H), 6.92 – 6.86 (m, 2H), 6.71 – 6.64 (m, 2H), 2.14 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.16, 157.67, 148.61, 142.35, 138.22, 137.22, 137.05, 130.01, 129.55, 129.08, 128.44, 128.10, 127.72, 126.65, 126.39, 125.98, 118.96, 115.59, 88.75, 82.98, 13.85. HRMS calcd for $C_{29}H_{22}IN_5NaO$ $[M+Na]^+$: 606.0767, found for: 606.0766.

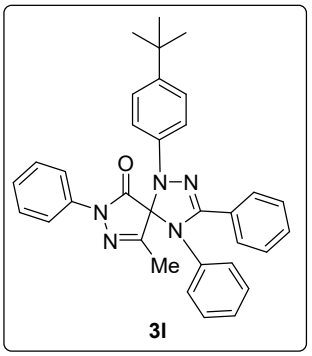
9-methyl-3,4,7-triphenyl-1-(4-(trifluoromethyl)phenyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3k)



3k

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1k** (43.5 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3k** as yellow solid after flash column chromatography (43.6 mg, 83% yield). M.p.: 251-253 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.66 (m, 2H), 7.52 – 7.44 (m, 4H), 7.41 – 7.32 (m, 3H), 7.28 (dd, *J* = 8.2, 6.6 Hz, 2H), 7.24 – 7.15 (m, 4H), 6.99 (dd, *J* = 8.0, 1.7 Hz, 4H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.84, 157.34, 149.10, 144.69, 137.14, 136.80, 130.18, 129.60, 129.11, 128.47, 128.17, 127.94, 126.93 (q, *J* = 3.8 Hz), 126.84, 126.18, 126.07, 124.54 (q, *J* = 270.9 Hz), 122.11 (q, *J* = 32.9 Hz), 118.96, 112.43, 88.35, 13.74. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -61.46. HRMS calcd for $C_{30}H_{22}F_3N_5NaO$ $[M+Na]^+$: 548.1674, found for: 548.1675.

1-(4-(tert-butyl)phenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3l)

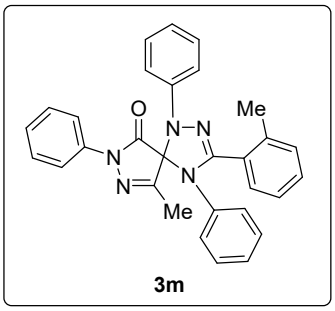


3l

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1l** (41.8 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3l** as yellow solid after flash column chromatography (44.1 mg, 86% yield). M.p.: 222-223 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.66 (m, 2H), 7.51 – 7.47 (m, 2H), 7.39 – 7.32 (m, 2H), 7.32 – 7.23 (m, 4H), 7.22 – 7.10 (m, 5H), 7.00 – 6.89 (m, 4H), 2.22 (s, 3H), 1.25 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.70, 158.27, 147.74, 143.83, 140.32, 137.48, 137.46, 129.63, 129.41, 129.00, 128.35, 128.00, 127.36, 126.85, 126.55, 126.34, 125.73, 119.02, 113.50, 89.27, 34.12, 31.45, 13.92. HRMS calcd for $C_{33}H_{31}N_5NaO$ $[M+Na]^+$: 536.2426, found for: 536.2427.

9-methyl-1,4,7-triphenyl-3-(o-tolyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-

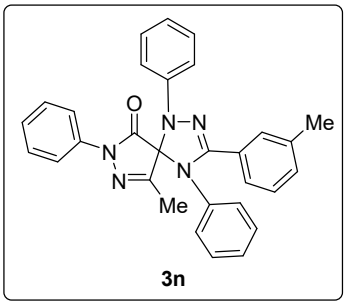
one (3m)



3m

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1m** (35.4 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3m** as yellow solid after flash column chromatography (40.1 mg, 85% yield). M.p.: 206-207 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.74 – 7.68 (m, 2H), 7.43 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.36 (t, *J* = 7.9 Hz, 2H), 7.26 – 7.18 (m, 4H), 7.17 – 7.11 (m, 2H), 7.10 – 7.03 (m, 3H), 6.99 (d, *J* = 8.0 Hz, 2H), 6.91 – 6.83 (m, 3H), 2.46 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.77, 157.88, 148.38, 143.22, 137.76, 137.45, 136.70, 130.93, 130.05, 129.86, 129.53, 129.33, 129.04, 127.02, 126.29, 125.86, 125.81, 125.63, 121.27, 118.99, 114.18, 88.74, 20.53, 13.96. HRMS calcd for $C_{30}H_{26}N_5O$ $[M+H]^+$: 472.2137, found for: 472.2138.

9-methyl-1,4,7-triphenyl-3-(m-tolyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3n)

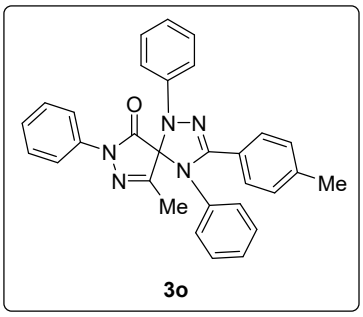


3n

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1n** (35.4 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3n** as yellow solid after flash column chromatography (42.9 mg, 91% yield). M.p.: 263-264 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.65 (m, 2H), 7.43 (s, 1H), 7.38 – 7.32 (m, 2H), 7.24 – 7.14 (m, 7H), 7.11 (d, *J* = 7.0 Hz, 2H), 7.02 – 6.95 (m, 4H), 6.87 (t, *J* = 7.3 Hz, 1H), 2.28 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.60, 158.08, 148.37, 142.88, 138.21, 137.43, 137.41, 130.62, 129.54, 129.40, 129.02, 128.70, 128.18, 127.42, 126.58, 125.79, 125.18, 121.12, 119.02, 113.90, 89.16, 21.39, 13.87. HRMS calcd for $C_{30}H_{26}N_5O$ $[M+H]^+$: 472.2137, found for: 472.2136.

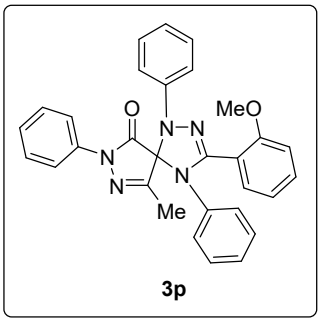
9-methyl-1,4,7-triphenyl-3-(p-tolyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-

one (3o)



The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1o** (35.4 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3o** as yellow solid after flash column chromatography (45.2 mg, 96% yield). M.p.: 273-274 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 – 7.65 (m, 2H), 7.40 – 7.32 (m, 4H), 7.23 – 7.17 (m, 4H), 7.17 – 7.10 (m, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 7.01 – 6.95 (m, 4H), 6.86 (t, *J* = 7.3 Hz, 1H), 2.30 (s, 3H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.62, 158.14, 148.28, 142.92, 139.99, 137.47, 137.43, 129.52, 129.41, 129.09, 129.01, 128.00, 127.42, 126.65, 125.78, 123.80, 121.04, 119.02, 113.86, 89.14, 21.47, 13.87. HRMS calcd for $C_{30}H_{25}N_5NaO$ $[M+Na]^+$: 494.1957, found for: 494.1958.

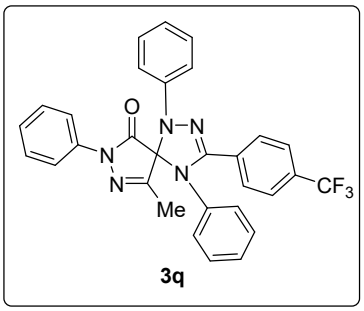
3-(2-methoxyphenyl)-9-methyl-1,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3p)



The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1p** (37.8 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3p** as yellow solid after flash column chromatography (47.3 mg, 97% yield). M.p.: 268-270 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.75 – 7.69 (m, 3H), 7.40 – 7.30 (m, 3H), 7.22 – 7.16 (m, 3H), 7.08 (dd, *J* = 8.3, 6.5 Hz, 2H), 7.04 – 6.97 (m, 4H), 6.90 – 6.84 (m, 3H), 6.70 (d, *J* = 8.3 Hz, 1H), 3.40 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.00, 158.13, 157.13, 147.60, 143.07, 137.57, 137.17, 131.86, 131.31, 129.44, 129.01, 128.91, 126.59, 125.74, 124.79, 121.08, 120.94, 119.03, 116.11, 114.22, 111.31, 88.86, 55.14, 13.84. HRMS calcd for $C_{30}H_{25}N_5NaO_2$ $[M+Na]^+$: 510.1906, found for: 510.1907.

9-methyl-1,4,7-triphenyl-3-(4-(trifluoromethyl)phenyl)-1,2,4,7,8-

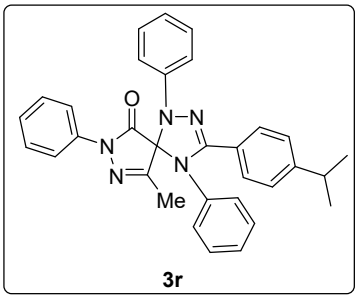
pentaazaspiro[4.4]nona-2,8-dien-6-one (3q)



3q

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1q** (43.5 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3q** as yellow solid after flash column chromatography (36.8 mg, 70% yield). M.p.: 222-224 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.36 (t, *J* = 7.9 Hz, 2H), 7.21 (qd, *J* = 8.7, 2.9 Hz, 6H), 6.99 (dd, *J* = 8.0, 5.0 Hz, 4H), 6.91 (t, *J* = 7.4 Hz, 1H), 2.23 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.22, 157.77, 146.75, 142.40, 137.27, 136.94, 131.27 (q, *J* = 32.7 Hz), 130.26, 129.70, 129.62, 129.03, 128.10, 127.90, 126.60, 125.90, 125.32 (q, *J* = 3.9 Hz), 121.55, 119.00, 113.86, 89.33, 13.85. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.85. HRMS calcd for $C_{30}H_{22}F_3N_5NaO$ $[M+Na]^+$: 548.1674, found for: 548.1673.

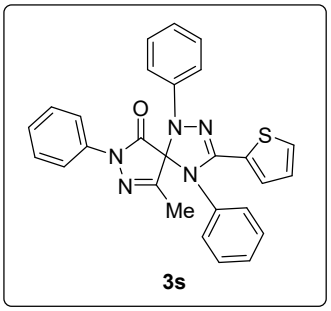
3-(4-isopropylphenyl)-9-methyl-1,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3r)



3r

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1r** (39.6 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3r** as yellow solid after flash column chromatography (48.4 mg, 97% yield). M.p.: 218-219 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.1 Hz, 2H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 7.9 Hz, 2H), 7.19 (td, *J* = 12.4, 11.2, 3.8 Hz, 6H), 7.12 (d, *J* = 8.2 Hz, 2H), 6.99 (d, *J* = 7.8 Hz, 4H), 6.86 (t, *J* = 7.3 Hz, 1H), 2.86 (p, *J* = 6.9 Hz, 1H), 2.20 (s, 3H), 1.20 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.62, 158.14, 150.85, 148.23, 142.90, 137.50, 137.44, 129.52, 129.43, 129.01, 128.04, 127.42, 126.65, 126.50, 125.78, 124.11, 121.02, 119.03, 113.83, 89.12, 34.03, 23.77, 13.84. HRMS calcd for $C_{32}H_{29}N_5NaO$ $[M+Na]^+$: 522.2270, found for: 522.2271.

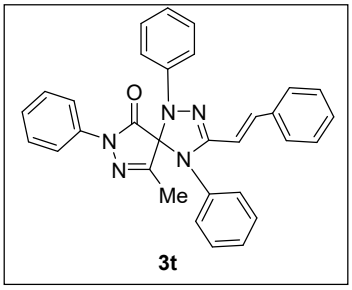
9-methyl-1,4,7-triphenyl-3-(thiophen-2-yl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3s)



3s

The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1s** (34.2 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3s** as yellow solid after flash column chromatography (45.0 mg, 97% yield). M.p.: 278-279 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.68 – 7.61 (m, 2H), 7.33 (t, *J* = 7.8 Hz, 2H), 7.30 – 7.25 (m, 4H), 7.19 (dtd, *J* = 14.7, 7.8, 7.0, 3.2 Hz, 6H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.90 – 6.80 (m, 2H), 6.71 (dd, *J* = 3.8, 1.1 Hz, 1H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.36, 157.91, 143.76, 142.72, 137.33, 136.19, 129.61, 129.56, 128.99, 128.69, 128.51, 128.38, 128.29, 127.82, 127.19, 125.80, 121.16, 119.00, 113.80, 89.48, 13.88. HRMS calcd for $C_{27}H_{21}N_5NaOS$ $[M+Na]^+$: 486.1365, found for: 486.1366.

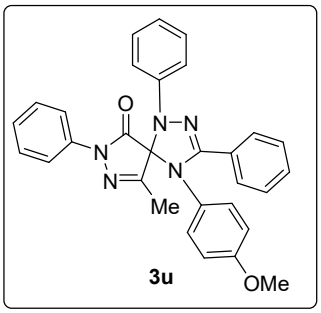
9-methyl-1,4,7-triphenyl-3-styryl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3t)



3t

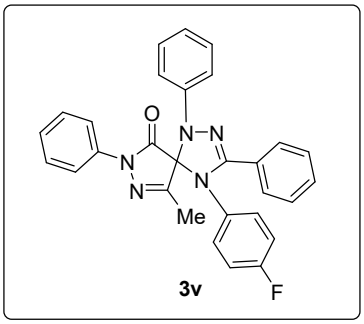
The reaction of pyrazolon-derived phenyl-ketimine **2a** (26.3 mg, 0.1 mmol) with tetrazole **1t** (37.2 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3t** as yellow solid after flash column chromatography (46.9 mg, 97% yield). M.p.: 253-254 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 8.1 Hz, 2H), 7.28 (s, 1H), 7.26 – 7.16 (m, 9H), 7.16 – 7.07 (m, 5H), 6.99 (d, *J* = 16.5 Hz, 1H), 6.90 (d, *J* = 8.1 Hz, 2H), 6.79 (t, *J* = 7.3 Hz, 1H), 6.38 (d, *J* = 16.5 Hz, 1H), 2.13 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.68, 157.88, 146.80, 142.64, 137.40, 136.15, 136.04, 135.78, 129.79, 129.60, 129.02, 128.97, 128.81, 128.21, 127.29, 127.03, 125.80, 121.18, 119.00, 113.80, 112.36, 89.10, 13.89. HRMS calcd for $C_{31}H_{25}N_5NaO$ $[M+Na]^+$: 506.1957, found for: 506.1955.

4-(4-methoxyphenyl)-9-methyl-1,3,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3u)



The reaction of pyrazolon-derived phenyl-ketimine **2b** (29.3 mg, 0.1 mmol) with tetrazole **1a** (33.3 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3u** as yellow solid after flash column chromatography (45.4 mg, 93% yield). M.p.: 265-267 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.72 – 7.66 (m, 2H), 7.52 – 7.46 (m, 2H), 7.39 – 7.16 (m, 8H), 6.97 (td, *J* = 7.4, 7.0, 1.7 Hz, 4H), 6.90 – 6.84 (m, 1H), 6.73 – 6.66 (m, 2H), 3.68 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.71, 158.76, 158.24, 148.49, 142.91, 137.44, 129.68, 129.66, 129.52, 128.98, 128.60, 128.32, 128.07, 126.69, 125.71, 120.92, 118.97, 114.60, 113.61, 89.36, 55.35, 13.86. HRMS calcd for $C_{30}H_{25}N_5NaO_2$ $[M+Na]^+$: 510.1906, found for: 510.1907.

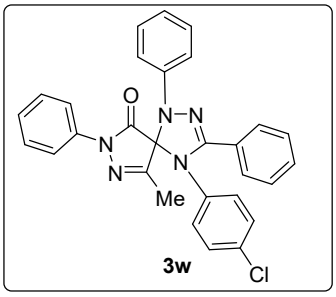
4-(4-fluorophenyl)-9-methyl-1,3,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3v)



The reaction of pyrazolon-derived phenyl-ketimine **2c** (28.2 mg, 0.1 mmol) with tetrazole **1a** (33.3 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3v** as yellow solid after flash column chromatography (42.4 mg, 89% yield). M.p.: 233-235 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 – 7.63 (m, 2H), 7.52 – 7.44 (m, 2H), 7.40 – 7.16 (m, 8H), 7.04 – 6.95 (m, 4H), 6.89 (t, *J* = 8.3 Hz, 3H), 2.26 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.24, 161.41 (d, *J* = 248.7 Hz), 158.19, 148.06, 142.74, 137.26, 133.30 (d, *J* = 3.3 Hz), 129.89, 129.57, 129.05, 128.83 (d, *J* = 8.7 Hz), 128.46, 128.02, 126.41, 125.89, 121.23, 118.91, 116.48 (d, *J* = 22.9 Hz), 113.76, 89.25, 13.80. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -112.62 (tt, *J* = 8.6, 4.8 Hz). HRMS calcd for $C_{29}H_{22}FN_5NaO$ $[M+Na]^+$: 498.1706, found for: 498.1707.

4-(4-chlorophenyl)-9-methyl-1,3,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

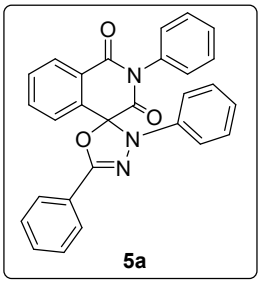
2,8-dien-6-one (3w)



The reaction of pyrazolon-derived phenyl-ketimine **2d** (29.8 mg, 0.1 mmol) with tetrazole **1a** (33.3 mg, 0.15 mmol) in MeCN (2 mL) led to compound **3w** as yellow solid after flash column chromatography (42.3 mg, 86% yield). M.p.: 217-219 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.73 – 7.67 (m, 2H), 7.51 – 7.45 (m, 2H), 7.41 – 7.26 (m, 5H), 7.25 – 7.18 (m, 3H), 7.18 – 7.13 (m, 2H), 7.02 – 6.96 (m, 2H), 6.93 – 6.86 (m, 3H), 2.22 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 167.26, 157.97, 147.76, 142.67, 137.26, 136.06, 133.09, 129.97, 129.65, 129.58, 129.09, 128.54, 128.00, 127.70, 126.38, 125.95, 121.40, 118.93, 113.95, 89.05, 13.82. HRMS calcd for $C_{29}H_{22}ClN_5NaO$ $[M+Na]^+$: 514.1411, found for: 514.1410.

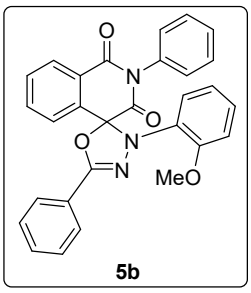
6.2 Characterization data of spirooxadiazolines

2,3',5'-triphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5a)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1a** (33.3 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5a** as yellow solid after flash column chromatography (40.1 mg, 90% yield). M.p.: 209-210 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.30 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.92 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.85 – 7.80 (m, 2H), 7.75 (td, *J* = 7.6, 1.4 Hz, 1H), 7.70 – 7.64 (m, 1H), 7.39 – 7.33 (m, 3H), 7.29 (td, *J* = 4.6, 3.8, 1.9 Hz, 2H), 7.21 – 7.12 (m, 3H), 6.98 – 6.91 (m, 1H), 6.89 – 6.82 (m, 2H), 6.79 – 6.67 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.03, 162.70, 152.65, 142.72, 136.54, 135.17, 133.76, 131.23, 130.90, 129.58, 129.38, 129.21, 128.95, 128.63, 128.21, 128.13, 126.74, 126.26, 124.64, 123.09, 117.11, 93.77. HRMS calcd for $C_{28}H_{19}N_3NaO_3$ $[M+Na]^+$: 468.1324, found for: 468.1322.

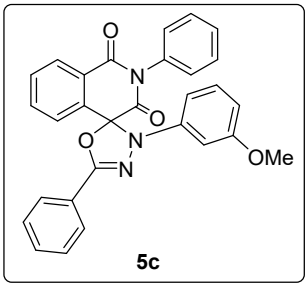
3'-(2-methoxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5b)



5b

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1b** (37.8 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5b** as yellow solid after flash column chromatography (39.5 mg, 83% yield). M.p.: 217-218 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 7.4 Hz, 1H), 7.96 – 7.89 (m, 2H), 7.60 – 7.50 (m, 4H), 7.49 – 7.35 (m, 6H), 7.10 (d, *J* = 7.5 Hz, 2H), 6.98 – 6.90 (m, 2H), 6.60 (dt, *J* = 6.7, 3.7 Hz, 1H), 3.33 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.68, 163.36, 153.41, 148.90, 136.13, 134.36, 133.88, 133.14, 130.87, 130.17, 129.21, 128.80, 128.61, 128.49, 128.35, 127.31, 126.85, 126.24, 124.72, 124.36, 121.71, 121.59, 111.06, 94.05, 55.02. HRMS calcd for $C_{29}H_{21}N_3NaO_4$ $[M+Na]^+$: 498.1430, found for: 498.1431.

3'-(3-methoxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5c)

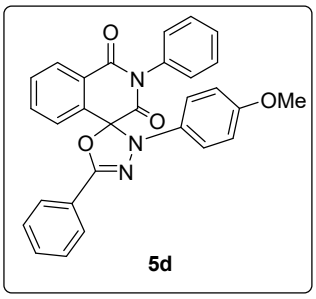


5c

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1c** (37.8 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5c** as yellow solid after flash column chromatography (44.2 mg, 93% yield). M.p.: 213-214 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.42 – 8.33 (m, 1H), 7.98 – 7.87 (m, 3H), 7.84 – 7.77 (m, 1H), 7.75 – 7.67 (m, 1H), 7.49 – 7.34 (m, 6H), 7.08 (t, *J* = 8.1 Hz, 1H), 6.93 (d, *J* = 7.1 Hz, 2H), 6.62 (t, *J* = 2.3 Hz, 1H), 6.54 (dd, *J* = 8.3, 2.4 Hz, 1H), 6.36 (dd, *J* = 8.1, 2.2 Hz, 1H), 3.70 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.03, 162.73, 160.66, 152.29, 143.86, 136.41, 135.23, 133.86, 131.32, 130.92, 130.09, 129.60, 129.27, 128.99, 128.64, 128.21, 128.19, 126.75, 126.25, 124.61, 108.65, 108.41, 102.48, 93.47, 55.22. HRMS calcd for $C_{29}H_{22}N_3O_4$ $[M+H]^+$: 476.1610, found for: 476.1611.

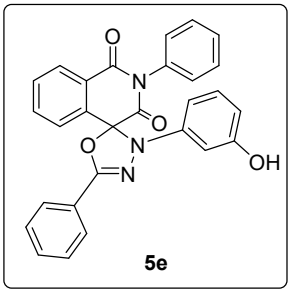
3'-(4-methoxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5d)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1d** (37.8 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5d** as yellow solid after flash column chromatography (46.1 mg, 97% yield). M.p.: 203-205 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.32 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.05 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.84 (td, *J* = 7.6, 1.4 Hz, 1H), 7.71 (td, *J* = 7.6, 1.3 Hz, 1H), 7.49 – 7.40 (m, 3H), 7.35 (dq, *J* = 5.2, 3.0 Hz, 3H), 6.88 – 6.83 (m, 2H), 6.80 – 6.76 (m, 2H), 6.68 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.35, 162.73, 156.99, 153.50, 136.97, 136.24, 135.02, 133.69, 131.04, 130.89, 129.30, 129.13, 128.89, 128.65, 128.15, 128.07, 126.79, 126.33, 124.75, 121.20, 114.65, 94.90, 55.62. HRMS calcd for $C_{29}H_{21}N_3NaO_4$ $[M+Na]^+$: 498.1430, found for: 498.1431.

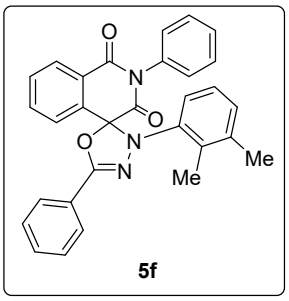
3'-(3-hydroxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5e)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1e** (35.7 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5e** as yellow solid after flash column chromatography (45.2 mg, 98% yield). M.p.: 233-234 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (d, *J* = 7.8 Hz, 1H), 7.97 – 7.84 (m, 3H), 7.79 (t, *J* = 7.6 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.41 (ddt, *J* = 20.9, 13.7, 6.8 Hz, 6H), 6.96 (dt, *J* = 16.0, 7.6 Hz, 3H), 6.60 (t, *J* = 2.3 Hz, 1H), 6.40 (dd, *J* = 8.1, 2.5 Hz, 1H), 6.27 (dd, *J* = 8.0, 2.2 Hz, 1H), 5.45 (s, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.14, 162.90, 156.95, 152.39, 143.86, 136.30, 135.28, 133.75, 131.36, 130.98, 130.28, 129.65, 129.33, 129.06, 128.67, 128.20, 128.15, 126.73, 126.08, 124.49, 110.04, 108.18, 104.17, 93.47. HRMS calcd for $C_{28}H_{19}N_3NaO_4$ $[M+Na]^+$: 484.1273, found for: 484.1272.

3'-(2,3-dimethylphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

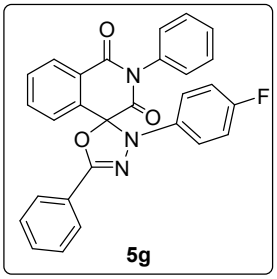
[1,3,4]oxadiazole]-1,3(2*H*)-dione (5f)



5f

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1f** (37.5 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5f** as yellow solid after flash column chromatography (19.4 mg, 41% yield). M.p.: 207-209 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (ddd, *J* = 15.5, 8.0, 1.3 Hz, 2H), 7.99 – 7.93 (m, 2H), 7.85 (td, *J* = 7.6, 1.4 Hz, 1H), 7.68 (td, *J* = 7.6, 1.2 Hz, 1H), 7.50 – 7.43 (m, 3H), 7.34 (tt, *J* = 4.7, 2.5 Hz, 3H), 7.19 – 7.06 (m, 3H), 6.53 (s, 2H), 2.14 (s, 3H), 1.47 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.76, 167.39, 162.33, 156.92, 145.64, 137.18, 136.23, 134.74, 133.69, 132.42, 132.17, 131.07, 130.18, 129.85, 129.52, 129.36, 128.80, 128.13, 128.03, 127.13, 126.04, 123.34, 122.19, 110.62, 20.31, 12.39. HRMS calcd for $C_{30}H_{24}N_3O_3$ $[M+H]^+$: 474.1818, found for: 474.1816.

3'-(4-fluorophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5g)

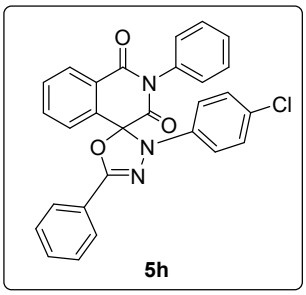


5g

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1g** (36.0 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5g** as yellow solid after flash column chromatography (36.6 mg, 79% yield). M.p.: 226-227 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.93 – 7.82 (m, 3H), 7.74 (td, *J* = 7.7, 1.3 Hz, 1H), 7.50 – 7.35 (m, 6H), 6.98 – 6.84 (m, 4H), 6.79 (s, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.95, 162.59, 159.37 (d, *J* = 243.2 Hz), 153.25, 139.12 (d, *J* = 2.6 Hz), 136.41, 135.19, 133.61, 131.18 (d, *J* = 25.7 Hz), 129.57, 129.27, 129.03, 128.67, 128.18, 128.14, 128.04, 126.80, 126.24, 124.50, 119.70 (d, *J* = 8.0 Hz), 116.08 (d, *J* = 22.6 Hz), 94.23. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -119.11. HRMS calcd for $C_{28}H_{18}FN_3NaO_3$ $[M+Na]^+$: 486.1230, found for: 486.1232.

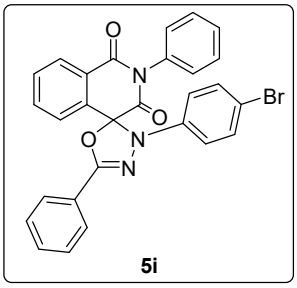
3'-(4-chlorophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5h)



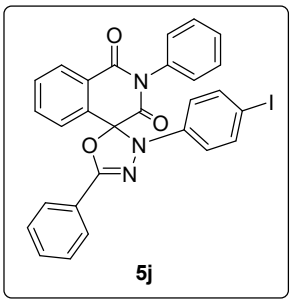
The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1h** (38.5 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5h** as yellow solid after flash column chromatography (40.8 mg, 85% yield). M.p.: 205-206 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.94 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.90 – 7.86 (m, 2H), 7.82 (td, *J* = 7.6, 1.4 Hz, 1H), 7.74 (td, *J* = 7.6, 1.3 Hz, 1H), 7.49 – 7.36 (m, 6H), 7.20 – 7.15 (m, 2H), 6.92 (d, *J* = 7.1 Hz, 2H), 6.88 – 6.81 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.72, 162.55, 152.64, 141.27, 135.86, 135.32, 133.68, 131.49, 131.09, 129.79, 129.35, 129.32, 129.09, 128.68, 128.17, 128.10, 127.79, 126.76, 126.20, 124.39, 117.67, 93.51. HRMS calcd for $C_{28}H_{18}ClN_3NaO_3$ $[M+Na]^+$: 502.0934, found for: 502.0933.

3'-(4-bromophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5i)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1i** (45.2 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5i** as yellow solid after flash column chromatography (40.9 mg, 78% yield). M.p.: 218-219 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.96 – 7.85 (m, 3H), 7.82 (td, *J* = 7.6, 1.4 Hz, 1H), 7.74 (td, *J* = 7.6, 1.3 Hz, 1H), 7.50 – 7.35 (m, 6H), 7.35 – 7.28 (m, 2H), 6.94 (d, *J* = 7.2 Hz, 2H), 6.83 – 6.75 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.66, 162.54, 152.57, 141.68, 135.75, 135.33, 133.67, 132.25, 131.52, 131.10, 129.83, 129.34, 129.10, 128.69, 128.15, 128.11, 126.75, 126.20, 124.37, 117.84, 115.08, 93.38. HRMS calcd for $C_{28}H_{18}BrN_3NaO_3$ $[M+Na]^+$: 546.0429, found for: 546.0430.

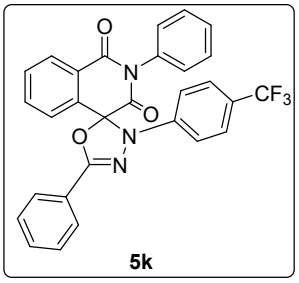
3'-(4-iodophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5j)



5j

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1j** (52.2 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5j** as yellow solid after flash column chromatography (42.9 mg, 75% yield). M.p.: 224-225 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.93 – 7.85 (m, 3H), 7.81 (td, *J* = 7.6, 1.5 Hz, 1H), 7.73 (td, *J* = 7.6, 1.3 Hz, 1H), 7.53 – 7.37 (m, 8H), 6.95 (d, *J* = 7.3 Hz, 2H), 6.71 – 6.65 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.63, 162.54, 152.49, 142.26, 138.13, 135.67, 135.35, 133.68, 131.54, 131.11, 129.85, 129.35, 129.11, 128.69, 128.13, 126.75, 126.18, 124.36, 123.79, 118.03, 93.25, 84.94. HRMS calcd for $C_{28}H_{18}IN_3NaO_3$ $[M+Na]^+$: 594.0291, found for: 594.0290.

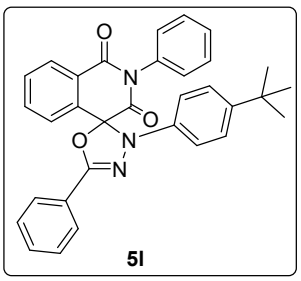
2,5'-diphenyl-3'-(4-(trifluoromethyl)phenyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5k)



5k

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1k** (43.5 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5k** as yellow solid after flash column chromatography (30.8 mg, 60% yield). M.p.: 209-211 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.87 (td, *J* = 7.9, 1.5 Hz, 3H), 7.78 (dtd, *J* = 21.5, 7.4, 1.5 Hz, 2H), 7.51 – 7.38 (m, 8H), 7.10 – 7.03 (m, 2H), 6.96 (d, *J* = 8.5 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.34, 162.47, 152.29, 144.71, 135.49, 135.02, 133.70, 131.76, 131.26, 130.10, 129.40, 129.20, 128.72, 128.11, 128.02, 126.78, 126.67 (q, *J* = 3.8 Hz), 126.19, 124.53 (q, *J* = 237.1 Hz), 124.16, 123.01, 114.26, 92.76. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -61.66. HRMS calcd for $C_{29}H_{18}F_3N_3NaO_3$ $[M+Na]^+$: 536.1198, found for: 536.1199.

3'-(4-(tert-butyl)phenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5l)

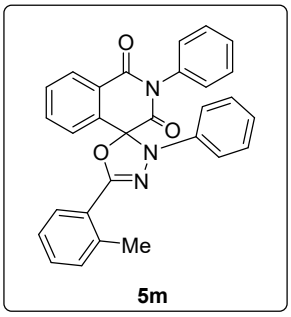


5l

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg,

0.1 mmol) with tetrazole **1l** (41.8 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5l** as yellow solid after flash column chromatography (32.1 mg, 64% yield). M.p.: 213-214 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.35 (dd, *J* = 7.9, 1.3 Hz, 1H), 8.04 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.84 (td, *J* = 7.6, 1.4 Hz, 1H), 7.72 (td, *J* = 7.6, 1.3 Hz, 1H), 7.48 – 7.39 (m, 3H), 7.32 (dd, *J* = 5.2, 2.0 Hz, 3H), 7.27 – 7.21 (m, 2H), 6.89 – 6.83 (m, 2H), 6.62 (s, 2H), 1.29 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.16, 162.74, 153.18, 147.08, 140.41, 137.08, 135.06, 133.73, 131.06, 130.84, 129.38, 129.09, 128.88, 128.62, 128.17, 128.12, 126.78, 126.29, 126.24, 124.77, 118.34, 94.44, 34.38, 31.44. HRMS calcd for $C_{32}H_{27}N_3NaO_3$ $[M+Na]^+$: 524.1950, found for: 524.1952.

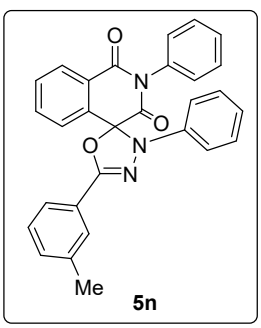
2,3'-diphenyl-5'-(o-tolyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5m)



5m

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1m** (35.4 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5m** as yellow solid after flash column chromatography (31.2 mg, 68% yield). M.p.: 206-207 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.03 – 7.96 (m, 1H), 7.87 – 7.69 (m, 3H), 7.40 – 7.26 (m, 6H), 7.23 – 7.19 (m, 2H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 7.9 Hz, 2H), 6.86 – 6.77 (m, 2H), 2.73 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.20, 162.75, 152.41, 142.81, 138.63, 136.77, 135.16, 133.80, 131.41, 131.17, 130.40, 129.60, 129.39, 129.23, 128.95, 128.34, 128.16, 128.13, 126.32, 125.82, 123.44, 122.98, 116.90, 92.67, 22.55. HRMS calcd for $C_{29}H_{21}N_3NaO_3$ $[M+Na]^+$: 482.1481, found for: 482.1482.

2,3'-diphenyl-5'-(m-tolyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5n)

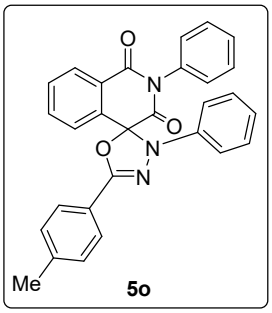


5n

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1n** (35.4 mg, 0.15 mmol) in 1,4-dioxane

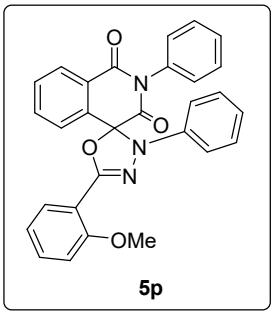
(2 mL) led to compound **5n** as yellow solid after flash column chromatography (33.5 mg, 73% yield). M.p.: 213-214 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.98 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.82 (td, *J* = 7.6, 1.4 Hz, 1H), 7.76 – 7.67 (m, 3H), 7.41 – 7.26 (m, 5H), 7.23 – 7.17 (m, 2H), 7.01 (t, *J* = 7.3 Hz, 1H), 6.95 – 6.89 (m, 2H), 6.82 (s, 2H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.06, 162.72, 152.82, 142.77, 138.43, 136.62, 135.17, 133.78, 131.75, 131.22, 129.57, 129.37, 129.21, 128.95, 128.57, 128.20, 128.15, 127.26, 126.25, 124.49, 123.95, 123.07, 117.13, 93.70, 21.35. HRMS calcd for $C_{29}H_{21}N_3NaO_3$ $[M+Na]^+$: 482.1481, found for: 482.1482.

2,3'-diphenyl-5'-(p-tolyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5o)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1o** (35.4 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5o** as yellow solid after flash column chromatography (34.5 mg, 75% yield). M.p.: 206-208 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 7.8 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.80 (dd, *J* = 10.3, 7.5 Hz, 3H), 7.71 (t, *J* = 7.6 Hz, 1H), 7.37 (dt, *J* = 7.1, 3.1 Hz, 3H), 7.22 (dt, *J* = 12.0, 5.1 Hz, 4H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.85 – 6.76 (m, 2H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.09, 162.75, 152.87, 142.87, 141.35, 136.66, 135.16, 133.81, 131.19, 129.55, 129.36, 129.21, 128.94, 128.22, 128.15, 126.74, 126.25, 123.01, 121.82, 117.13, 93.66, 21.66. HRMS calcd for $C_{29}H_{21}N_3NaO_3$ $[M+Na]^+$: 482.1481, found for: 482.1480.

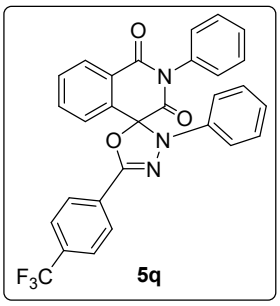
5'-(2-methoxyphenyl)-2,3'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5p)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1p** (38.0 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5p** as yellow solid after flash

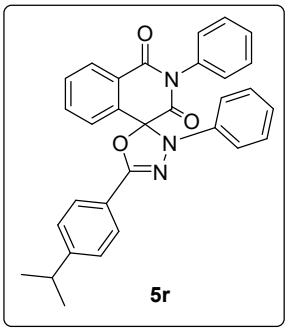
column chromatography (38.0 mg, 80% yield). M.p.: 219-221 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 – 8.33 (m, 1H), 8.05 – 8.00 (m, 1H), 7.84 – 7.75 (m, 2H), 7.73 – 7.67 (m, 1H), 7.46 – 7.33 (m, 4H), 7.24 – 7.17 (m, 2H), 7.00 (dd, *J* = 9.6, 6.9 Hz, 3H), 6.96 – 6.91 (m, 2H), 6.82 (s, 2H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.22, 162.82, 158.28, 150.71, 142.93, 136.89, 135.10, 133.87, 132.16, 131.07, 129.89, 129.48, 129.28, 129.19, 128.89, 128.24, 128.16, 126.33, 123.01, 120.49, 117.31, 113.60, 111.84, 92.66, 56.23. HRMS calcd for $C_{29}H_{21}N_3NaO_4$ $[M+Na]^+$: 498.1430, found for: 498.1429.

2,3'-diphenyl-5'-(4-(trifluoromethyl)phenyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5q)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1q** (43.5 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5q** as yellow solid after flash column chromatography (28.8 mg, 56% yield). M.p.: 206-207 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.39 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.04 – 7.95 (m, 3H), 7.84 (td, *J* = 7.6, 1.4 Hz, 1H), 7.75 (td, *J* = 7.6, 1.3 Hz, 1H), 7.69 (d, *J* = 8.3 Hz, 2H), 7.42 – 7.33 (m, 3H), 7.25 – 7.20 (m, 2H), 7.04 (t, *J* = 7.4 Hz, 1H), 6.96 – 6.90 (m, 2H), 6.83 (s, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.84, 162.54, 151.43, 142.24, 136.08, 135.26, 133.64, 132.32 (q, *J* = 32.7 Hz), 131.46, 129.72, 129.47, 129.27, 129.05, 128.15, 128.08, 128.02, 126.88, 126.28, 125.65 (q, *J* = 3.8 Hz), 123.78 (q, *J* = 272.3 Hz), 123.45, 117.13, 94.13. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -62.89. HRMS calcd for $C_{29}H_{18}F_3N_3NaO_3$ $[M+Na]^+$: 536.1198, found for: 536.1199.

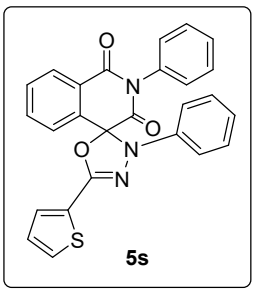
5'-(4-isopropylphenyl)-2,3'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5r)



The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1r** (40.0 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5r** as yellow solid after

flash column chromatography (33.6 mg, 69% yield). M.p.: 217-219 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 7.9, 1.4 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.85 – 7.78 (m, 3H), 7.71 (td, *J* = 7.6, 1.3 Hz, 1H), 7.36 (dd, *J* = 5.9, 1.7 Hz, 3H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.25 – 7.18 (m, 2H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.82 (s, 2H), 2.94 (hept, *J* = 6.9 Hz, 1H), 1.26 (d, *J* = 6.9 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.05, 162.76, 152.84, 152.24, 142.88, 136.69, 135.15, 133.82, 131.18, 129.54, 129.36, 129.20, 128.93, 128.20, 128.16, 126.89, 126.78, 126.26, 123.01, 122.17, 117.15, 93.65, 34.26, 23.81. HRMS calcd for $C_{31}H_{25}N_3NaO_3$ $[M+Na]^+$: 510.1794, found for: 510.1795.

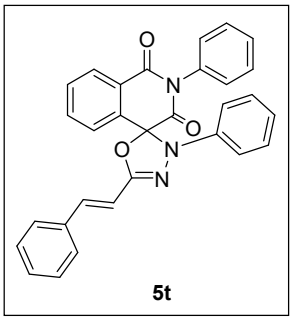
2,3'-diphenyl-5'-(thiophen-2-yl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione (5s)



5s

The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1s** (34.2 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5s** as yellow solid after flash column chromatography (39.3 mg, 87% yield). M.p.: 220-222 ℃. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.36 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.03 – 7.99 (m, 1H), 7.83 (td, *J* = 7.6, 1.4 Hz, 1H), 7.72 (td, *J* = 7.7, 1.3 Hz, 1H), 7.55 (dd, *J* = 3.7, 1.3 Hz, 1H), 7.45 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.36 (dd, *J* = 5.3, 2.0 Hz, 3H), 7.21 (t, *J* = 8.0 Hz, 2H), 7.08 (dd, *J* = 5.0, 3.6 Hz, 1H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.93 – 6.87 (m, 2H), 6.80 (s, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.84, 162.64, 149.33, 142.64, 136.24, 135.19, 133.71, 131.33, 129.58, 129.39, 129.22, 129.17, 128.97, 128.27, 128.13, 127.71, 126.32, 126.16, 123.33, 117.40, 93.94. HRMS calcd for $C_{26}H_{17}N_3NaO_3S$ $[M+Na]^+$: 474.0888, found for: 474.0889.

2,3'-diphenyl-5'-styryl-1H,3'H-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2H)-dione (5t)



5t

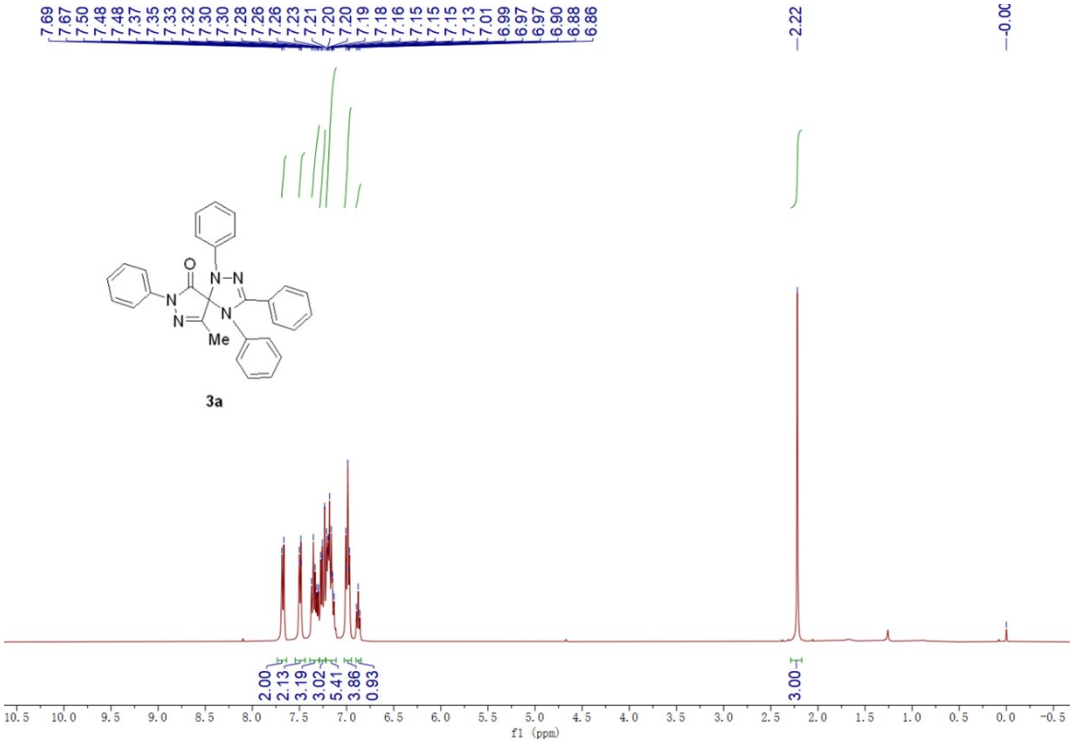
The reaction of isoquinoline-1,3,4(2*H*)-triones **4a** (25.1 mg, 0.1 mmol) with tetrazole **1s** (37.2 mg, 0.15 mmol) in 1,4-dioxane (2 mL) led to compound **5t** as yellow solid after

flash column chromatography (42.4 mg, 90% yield). M.p.: 240-241 °C. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.37 (d, *J* = 7.9 Hz, 1H), 7.95 (d, *J* = 7.8 Hz, 1H), 7.82 (t, *J* = 7.6 Hz, 1H), 7.72 (t, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 2H), 7.40 – 7.30 (m, 7H), 7.22 – 7.16 (m, 3H), 7.00 (t, *J* = 7.3 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 3H), 6.79 (d, *J* = 16.3 Hz, 1H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.02, 162.67, 152.81, 142.29, 136.84, 136.43, 135.32, 135.26, 133.78, 131.32, 129.64, 129.43, 129.36, 129.27, 129.02, 128.93, 128.21, 128.15, 127.30, 126.22, 123.07, 116.79, 110.63, 93.37. HRMS calcd for $C_{30}H_{21}N_3NaO_3$ $[M+Na]^+$: 494.1481, found for: 494.1480.

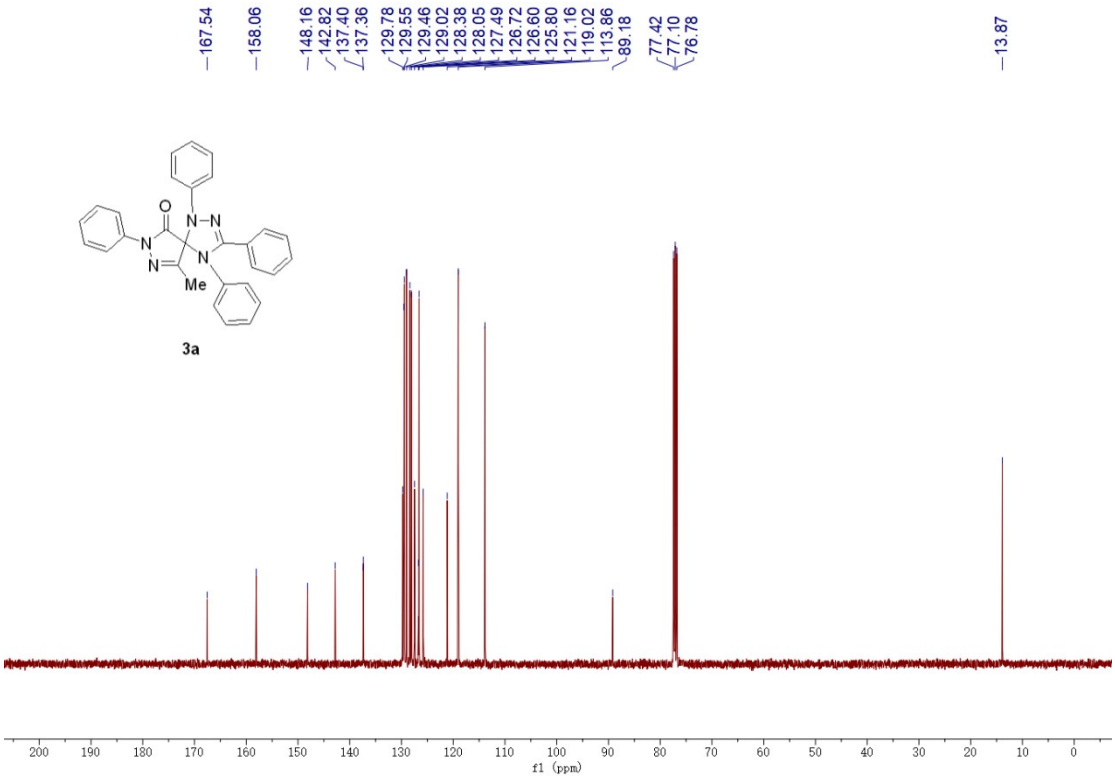
7. NMR spectra

9-methyl-1,3,4,7-tetraphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3a)

^{1}H NMR ($CDCl_3$, 400 MHz)

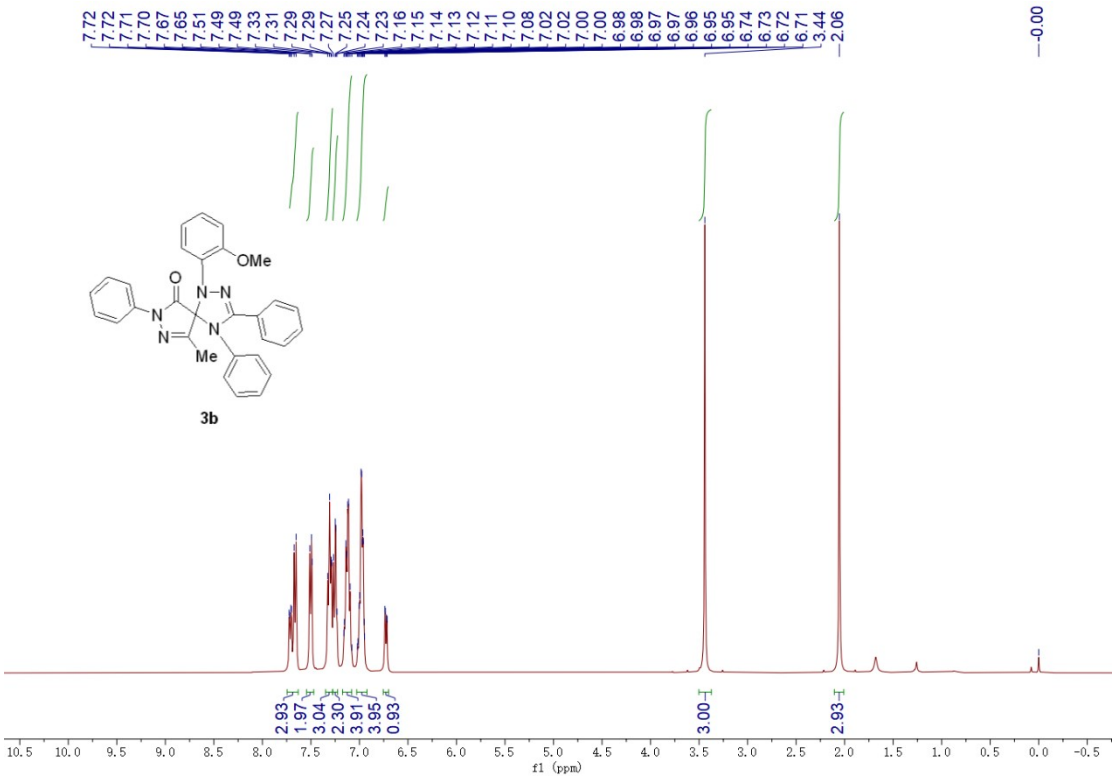


^{13}C NMR ($CDCl_3$, 100 MHz)

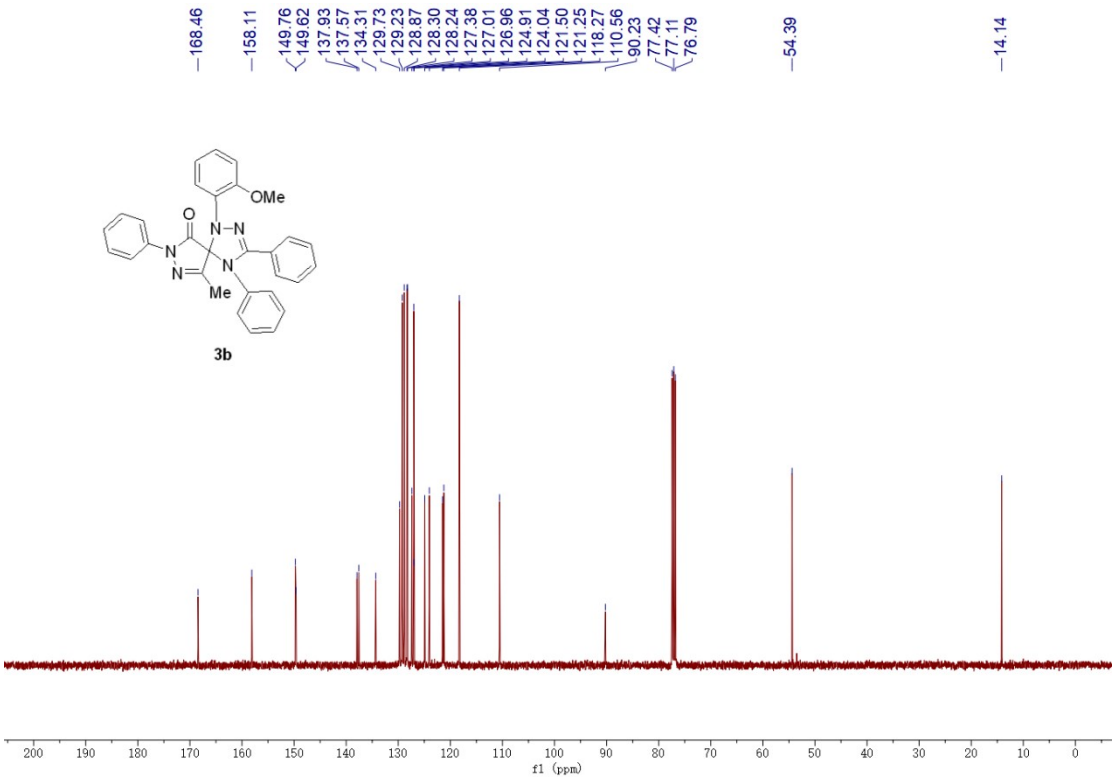


1-(2-methoxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3b)

^{1}H NMR ($CDCl_3$, 400 MHz)

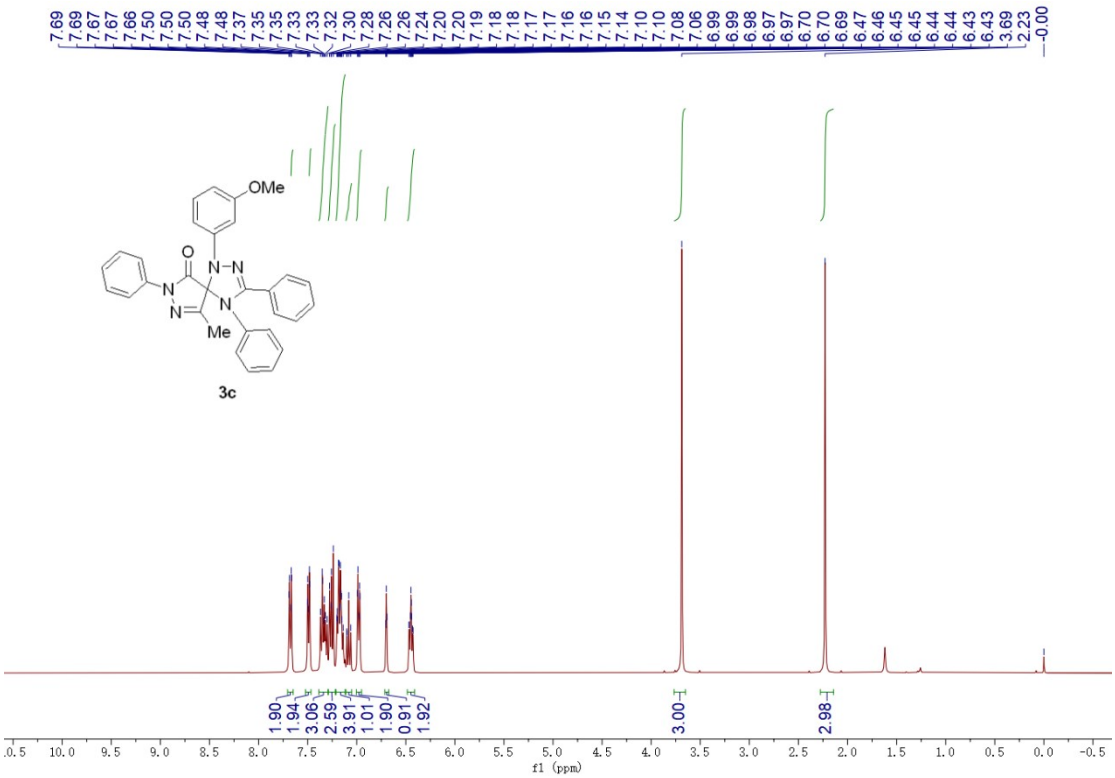


^{13}C NMR ($CDCl_3$, 100 MHz)

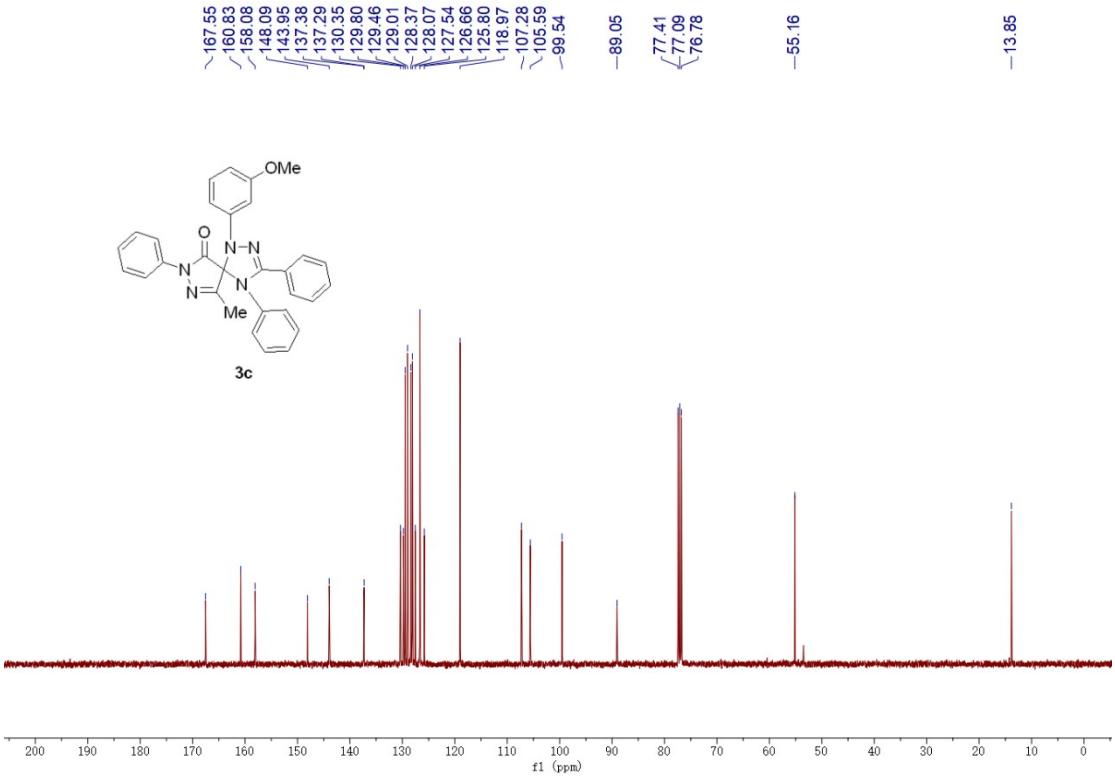


1-(3-methoxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3c)

^{1}H NMR ($CDCl_3$, 400 MHz)

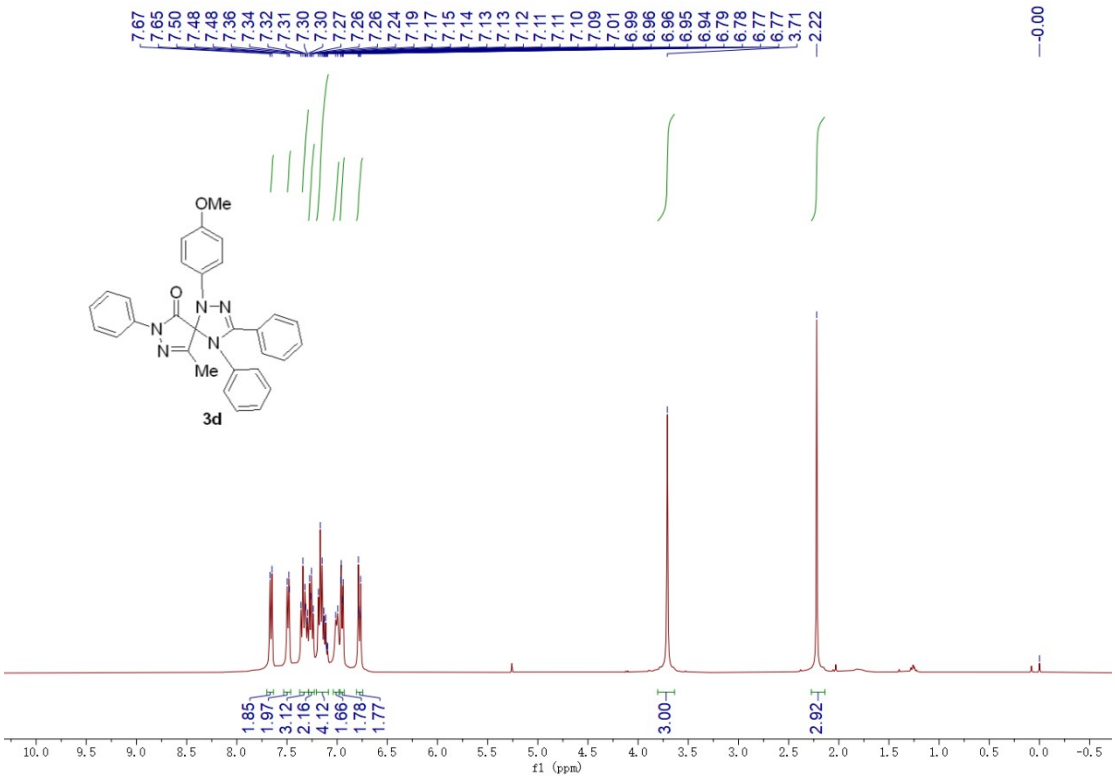


^{13}C NMR ($CDCl_3$, 100 MHz)

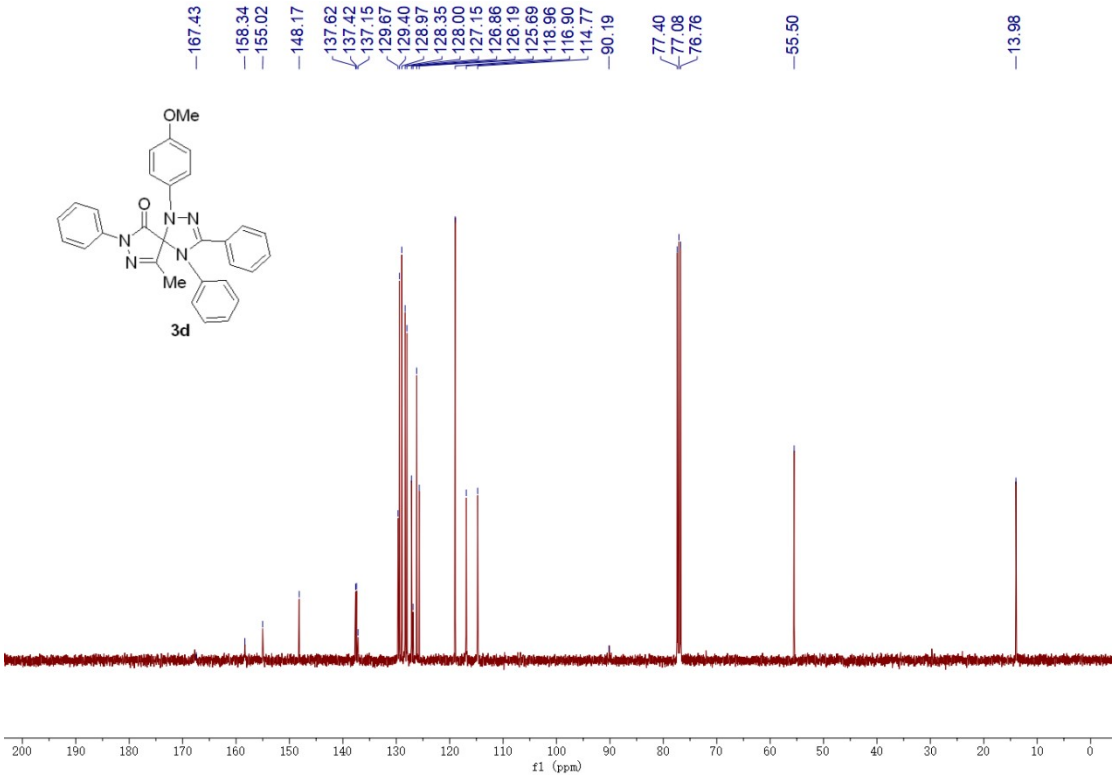


1-(4-methoxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3d)

^{1}H NMR ($CDCl_3$, 400 MHz)

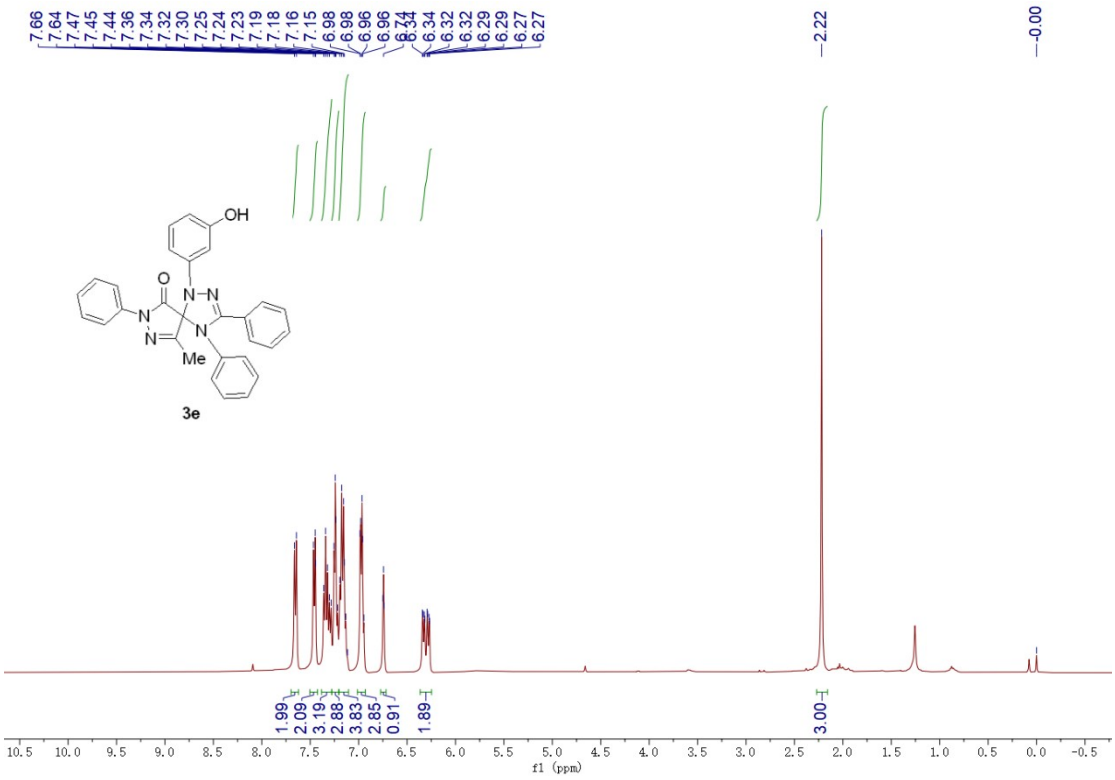


^{13}C NMR ($CDCl_3$, 100 MHz)

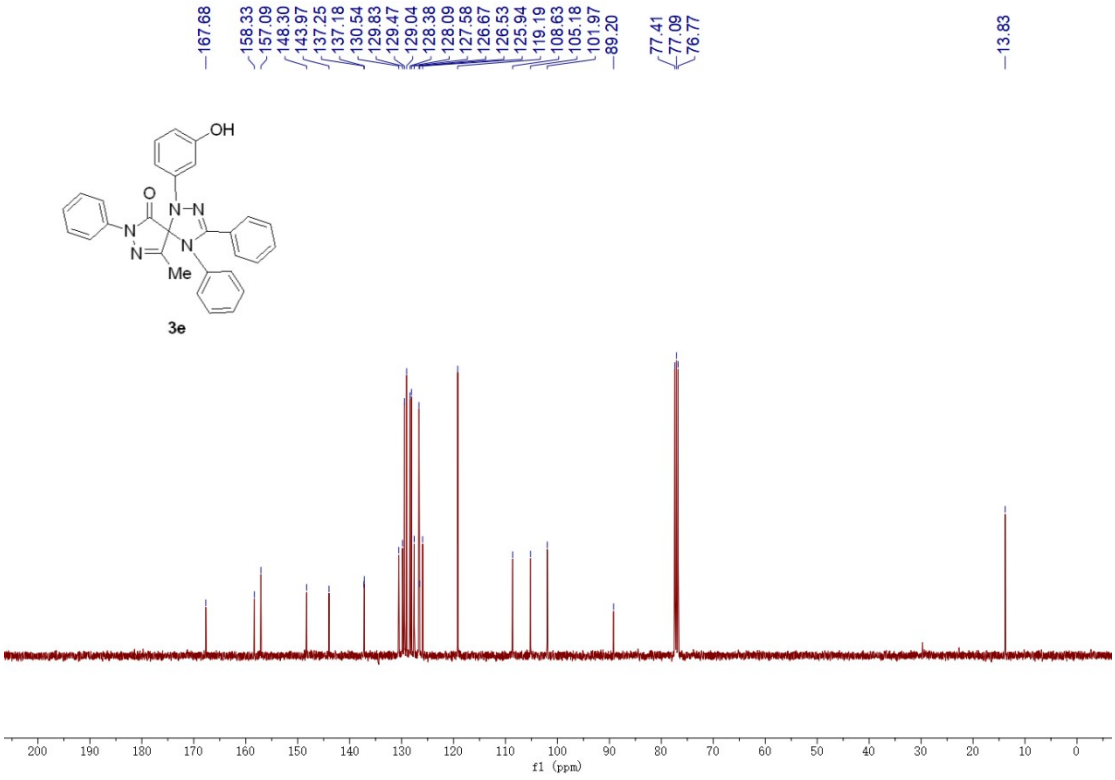


1-(3-hydroxyphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3e)

^{1}H NMR ($CDCl_3$, 400 MHz)

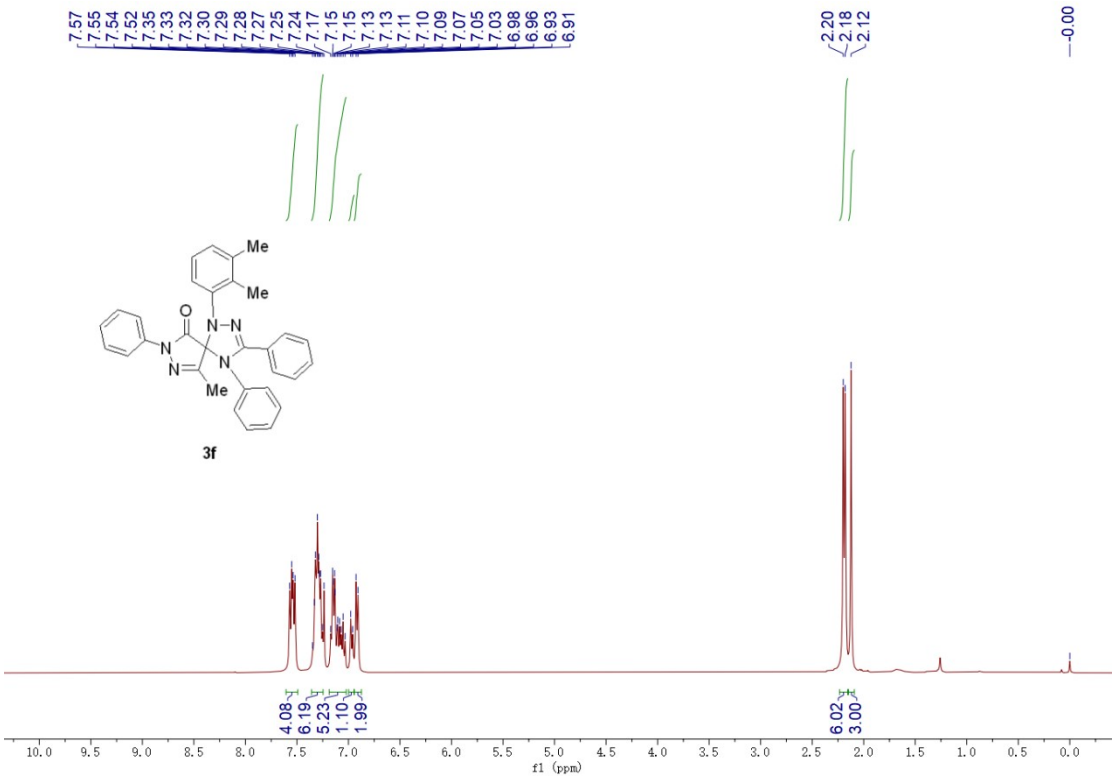


^{13}C NMR ($CDCl_3$, 100 MHz)

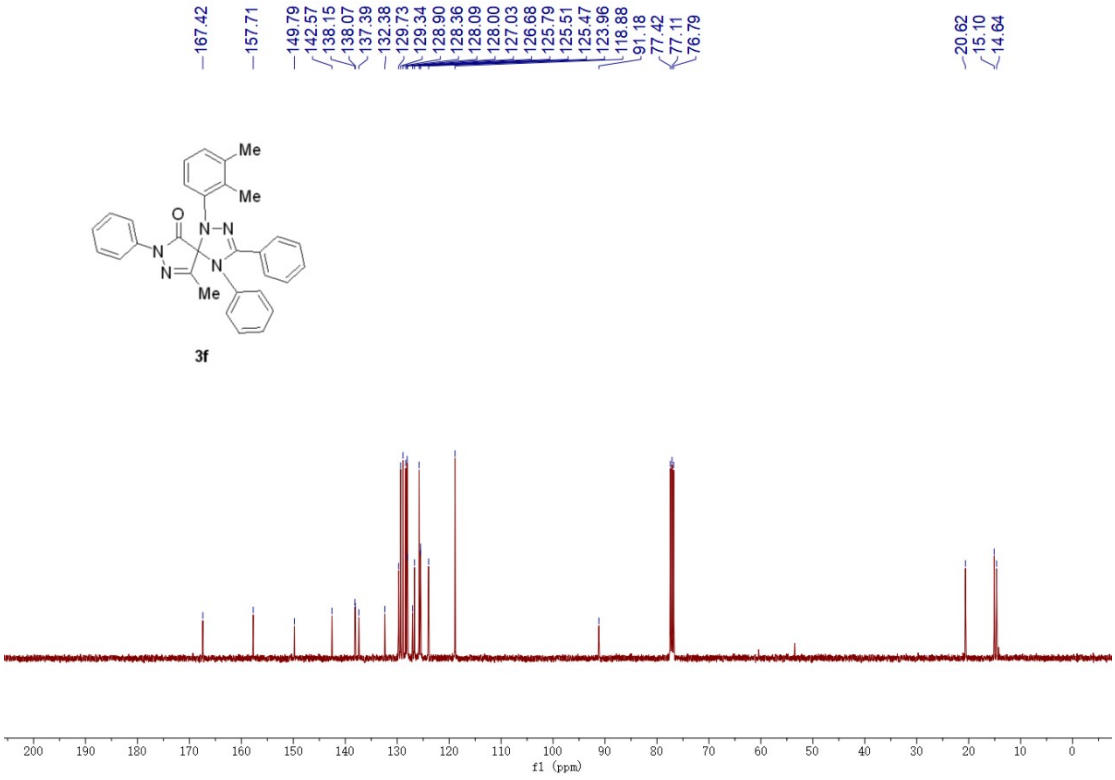


1-(2,3-dimethylphenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3f)

^{1}H NMR ($CDCl_3$, 400 MHz)

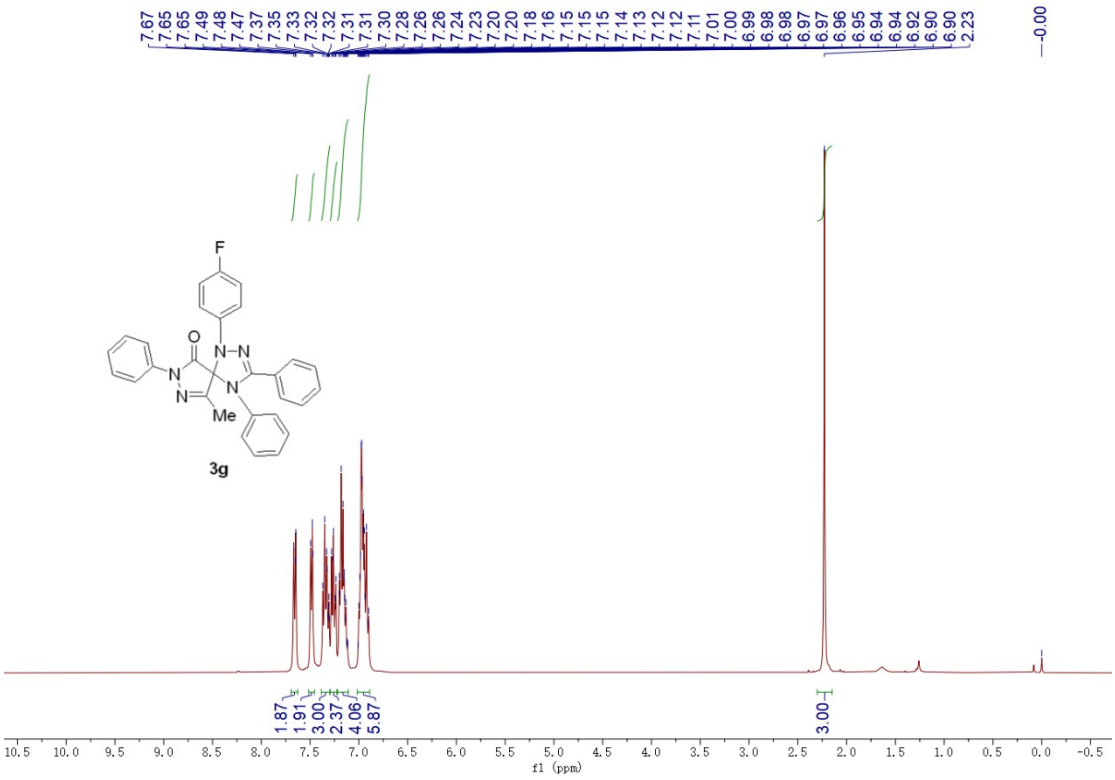


^{13}C NMR ($CDCl_3$, 100 MHz)

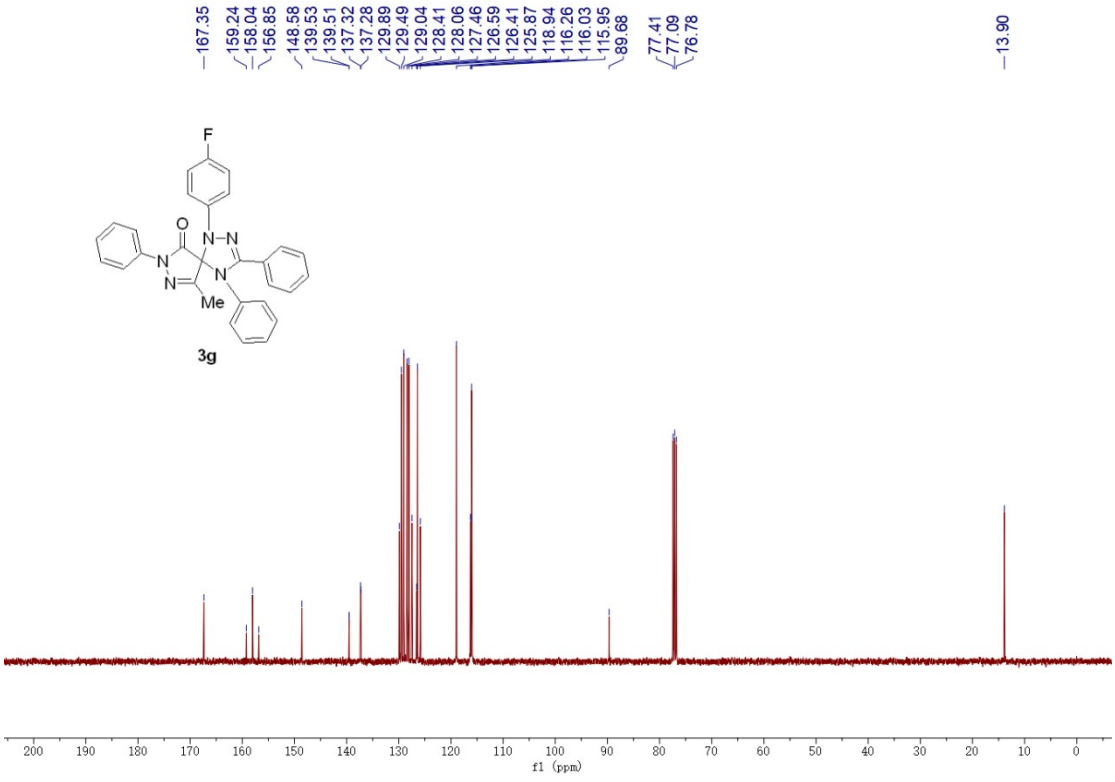


1-(4-fluorophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one (3g)

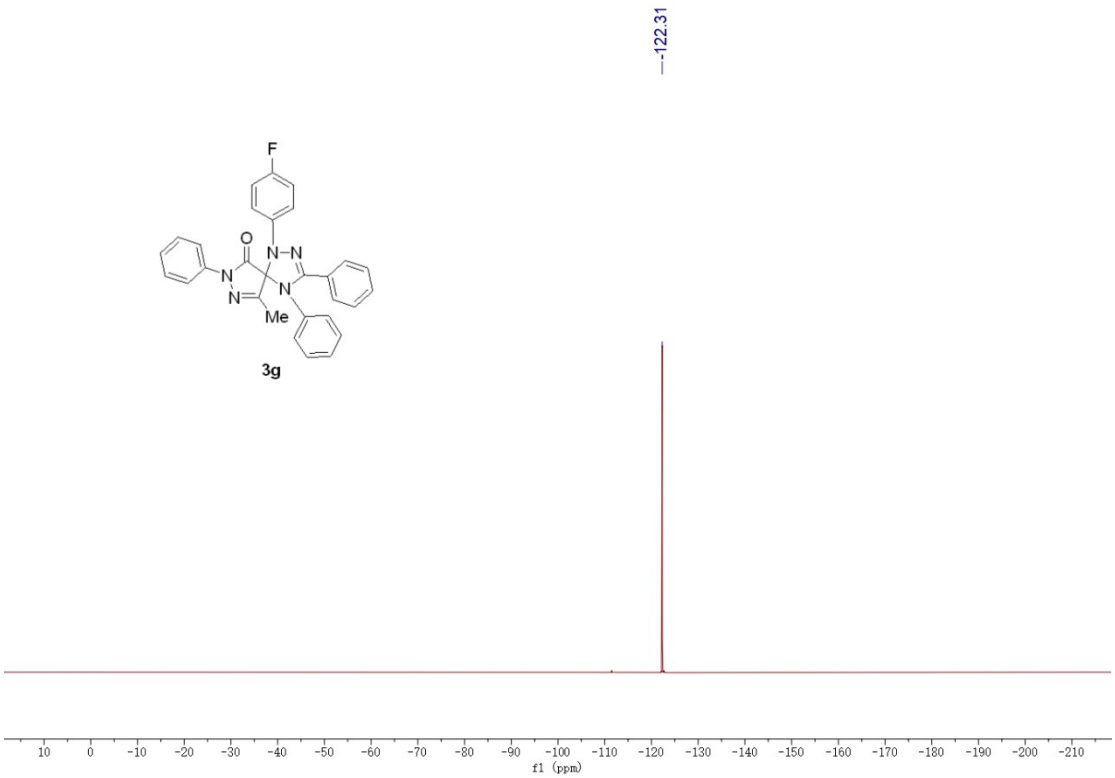
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



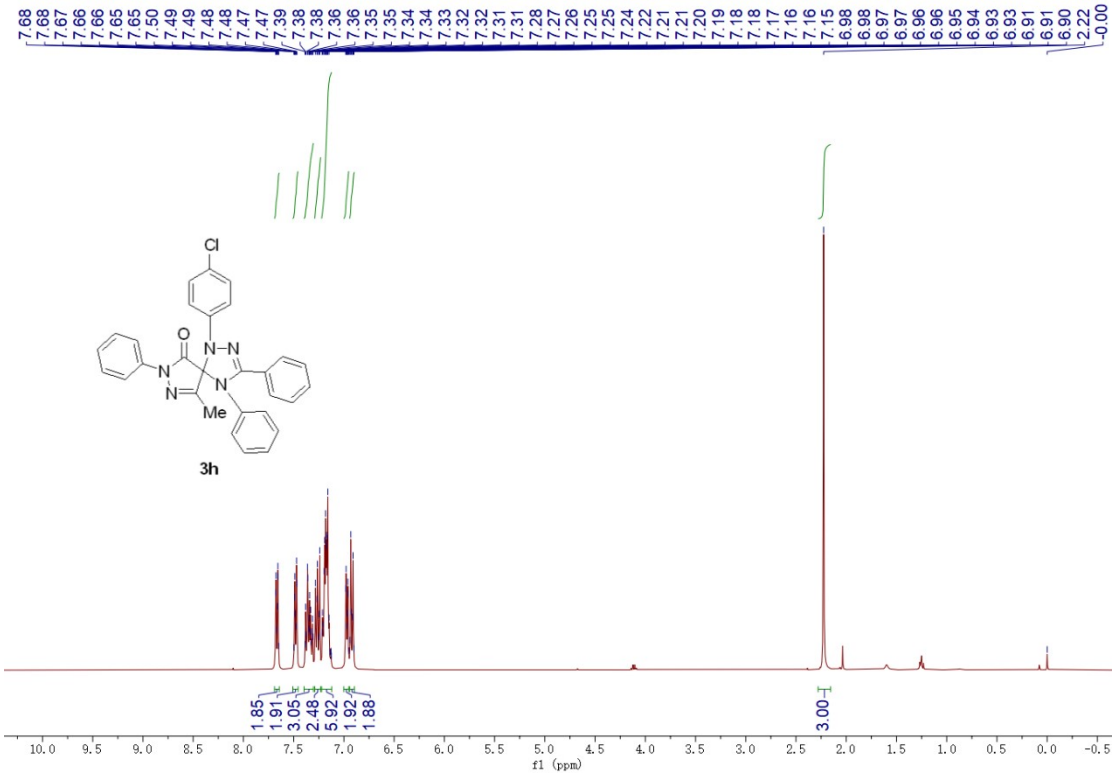
^{19}F NMR ($CDCl_3$, 376 MHz)



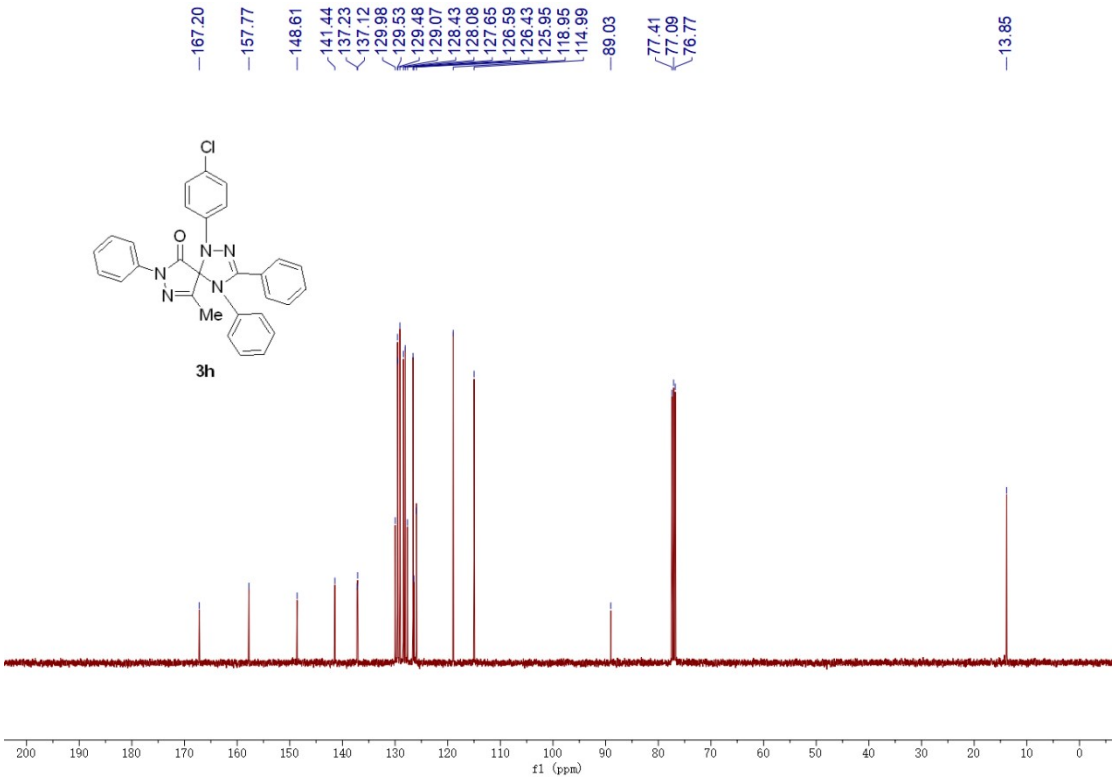
1-(4-chlorophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3h)

^{1}H NMR ($CDCl_3$, 400 MHz)



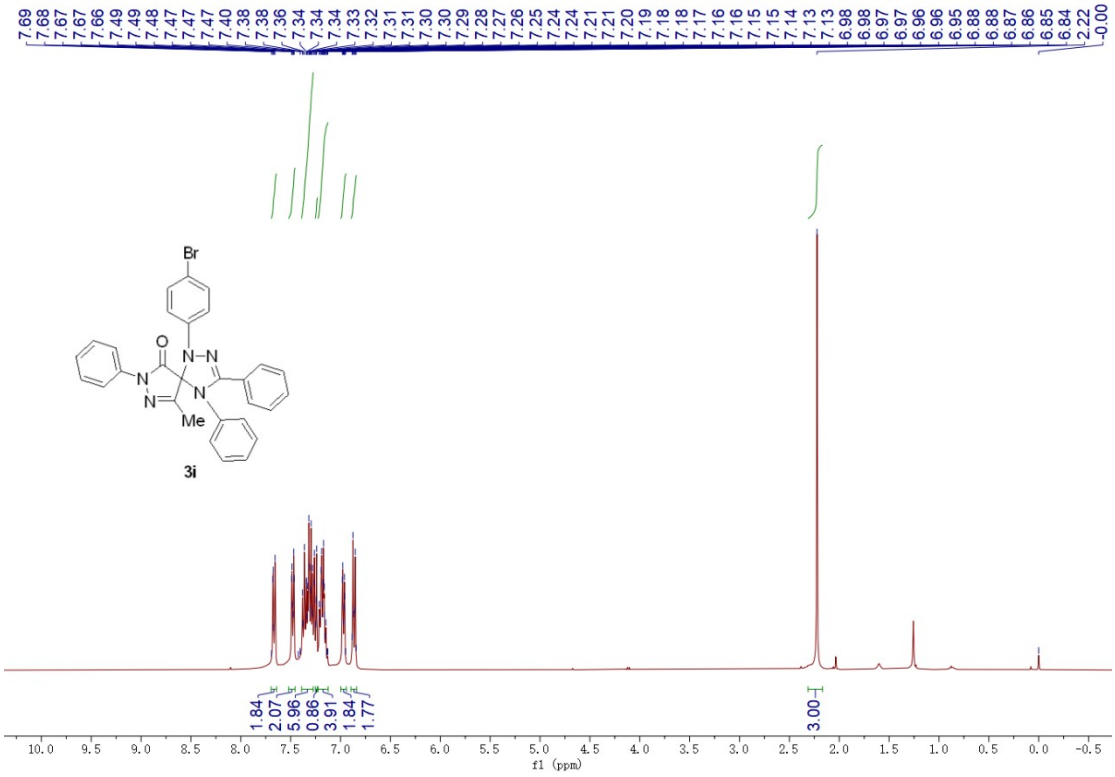
^{13}C NMR ($CDCl_3$, 100 MHz)



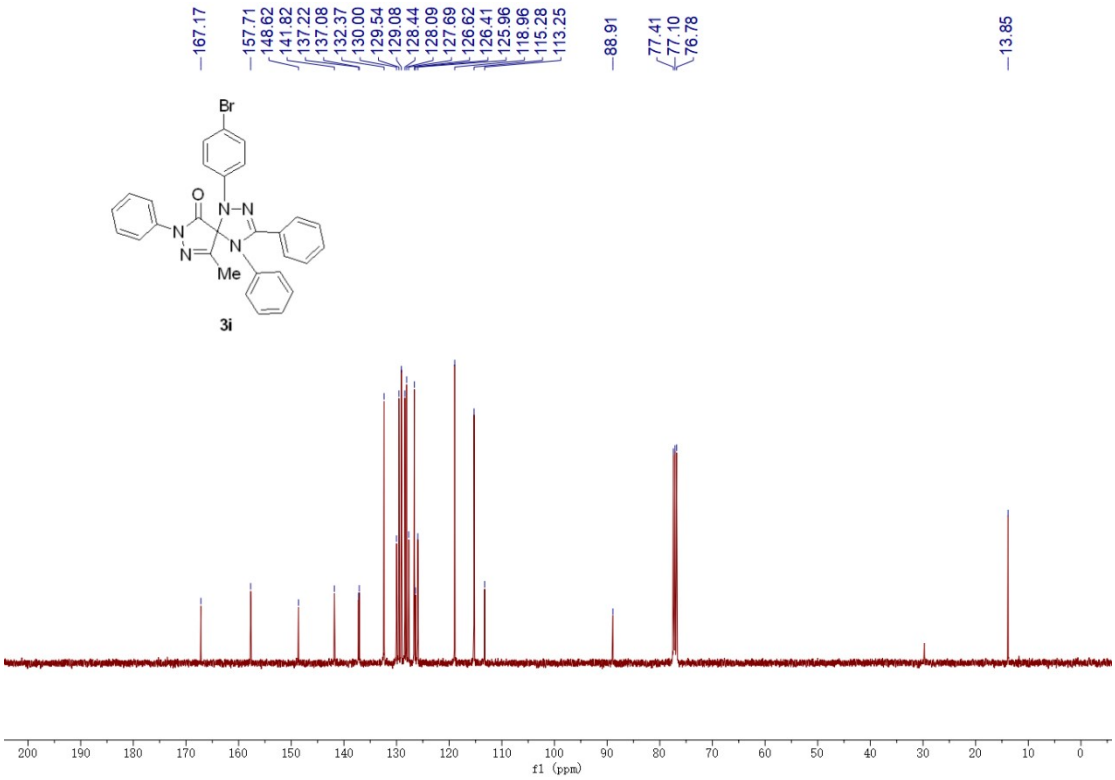
1-(4-bromophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3i)

^{1}H NMR ($CDCl_3$, 400 MHz)



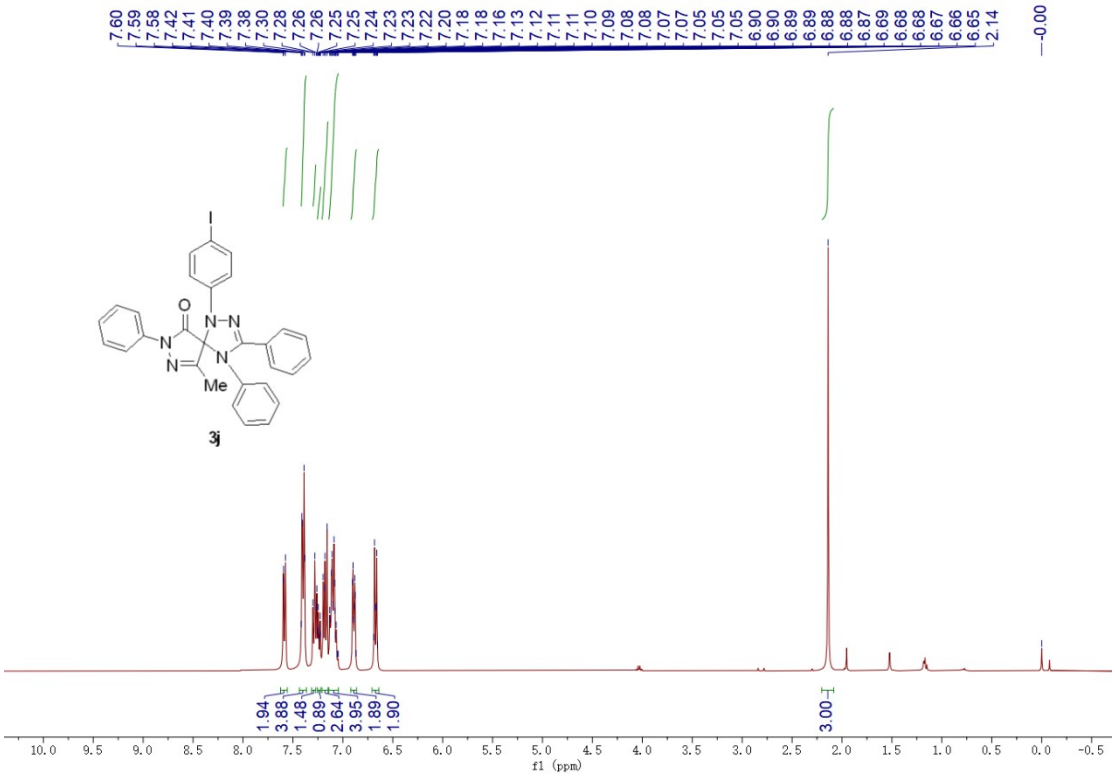
^{13}C NMR ($CDCl_3$, 100 MHz)



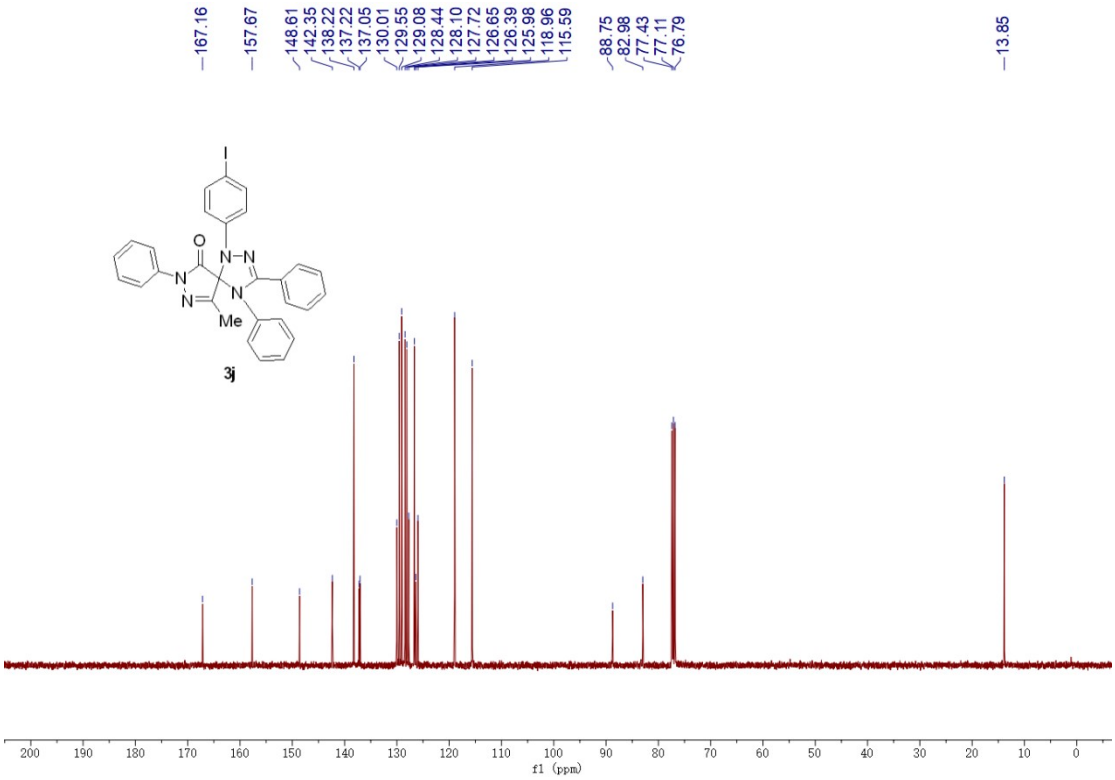
1-(4-iodophenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-

dien-6-one (3j)

^{1}H NMR ($CDCl_3$, 400 MHz)



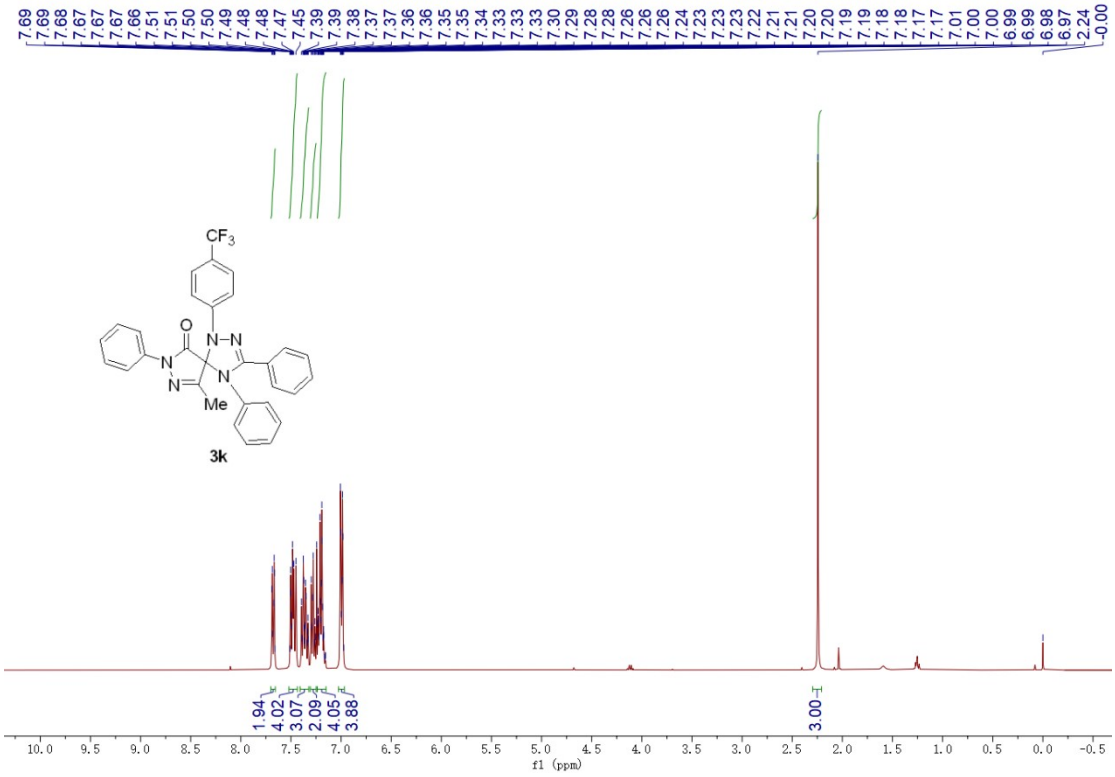
^{13}C NMR ($CDCl_3$, 100 MHz)



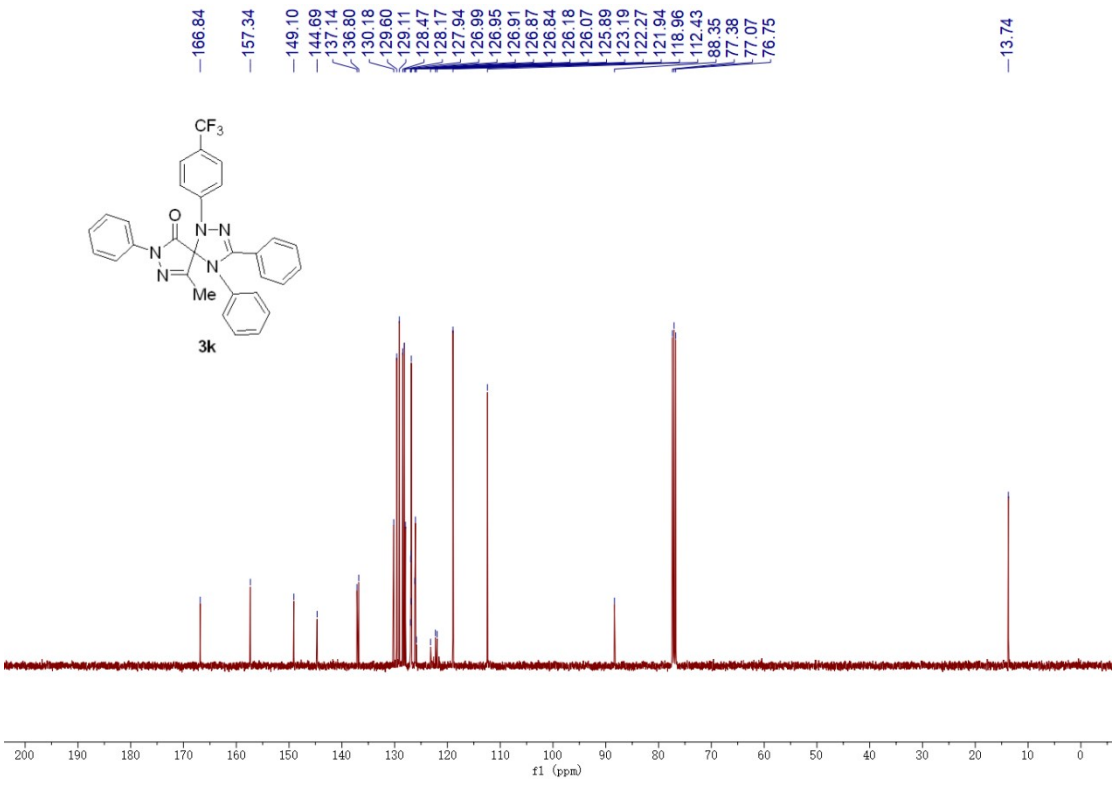
9-methyl-3,4,7-triphenyl-1-(4-(trifluoromethyl)phenyl)-1,2,4,7,8-

pentaazaspiro[4.4]nona-2,8-dien-6-one (3k)

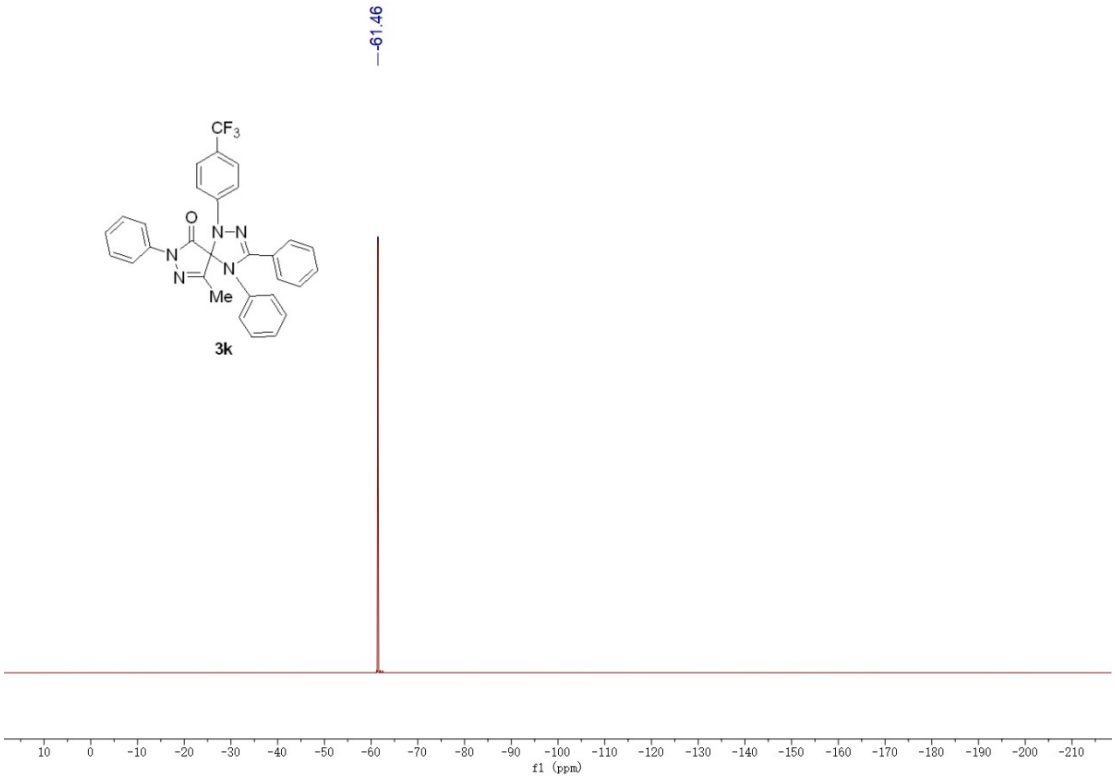
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



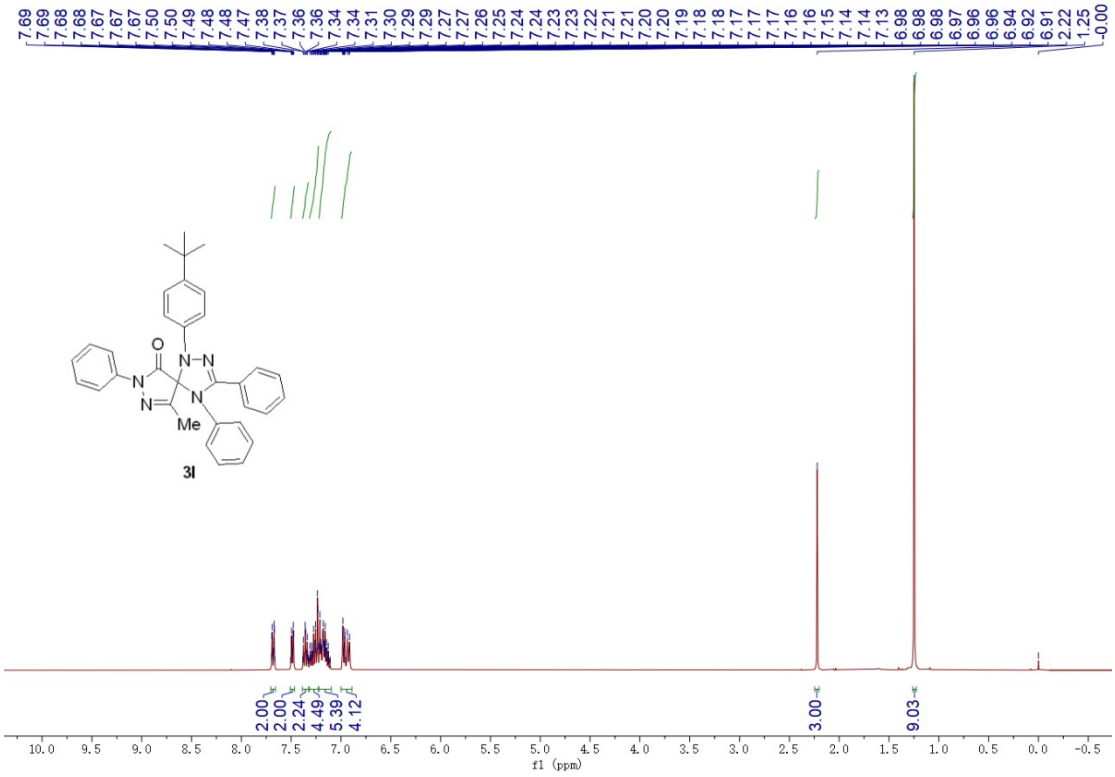
^{19}F NMR ($CDCl_3$, 376 MHz)



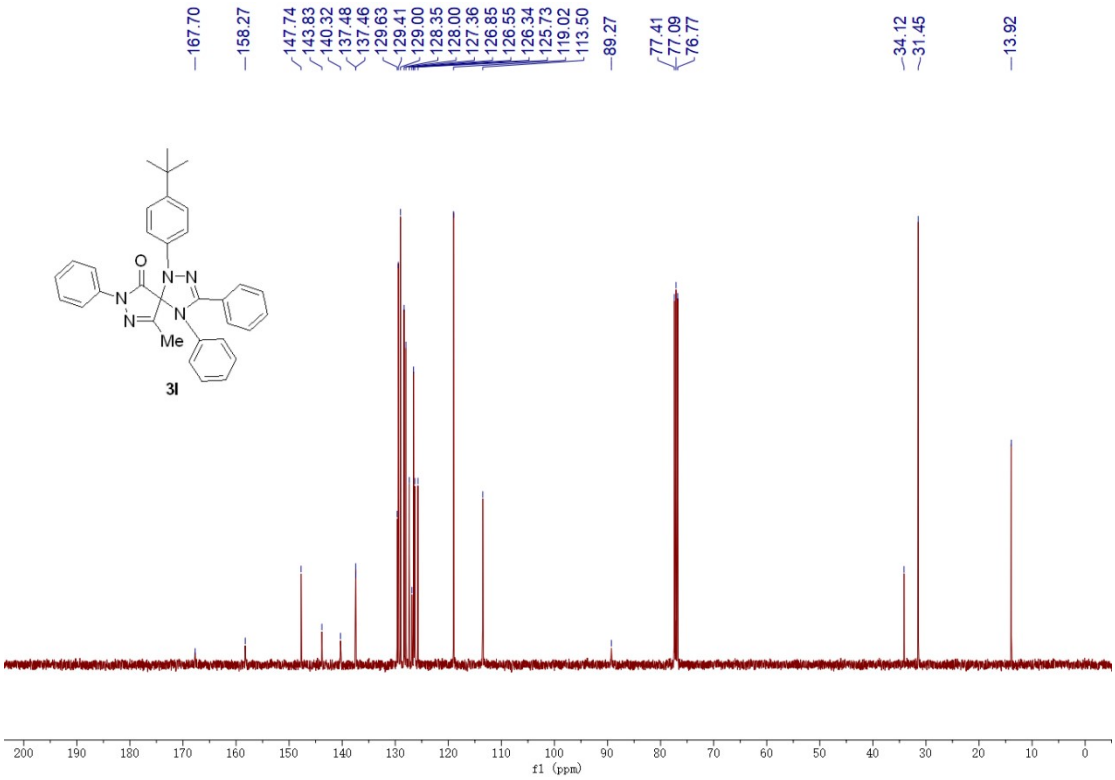
1-(4-(tert-butyl)phenyl)-9-methyl-3,4,7-triphenyl-1,2,4,7,8-

pentaazaspiro[4.4]nona-2,8-dien-6-one (3l)

^{1}H NMR ($CDCl_3$, 400 MHz)



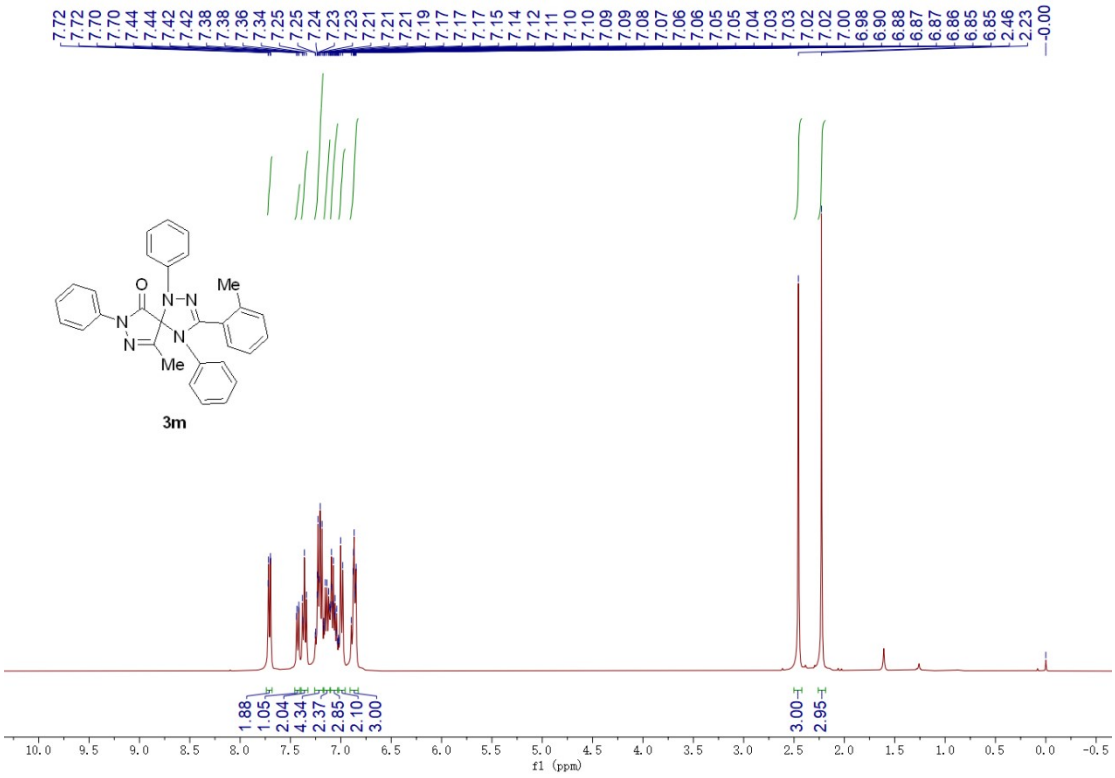
^{13}C NMR ($CDCl_3$, 100 MHz)



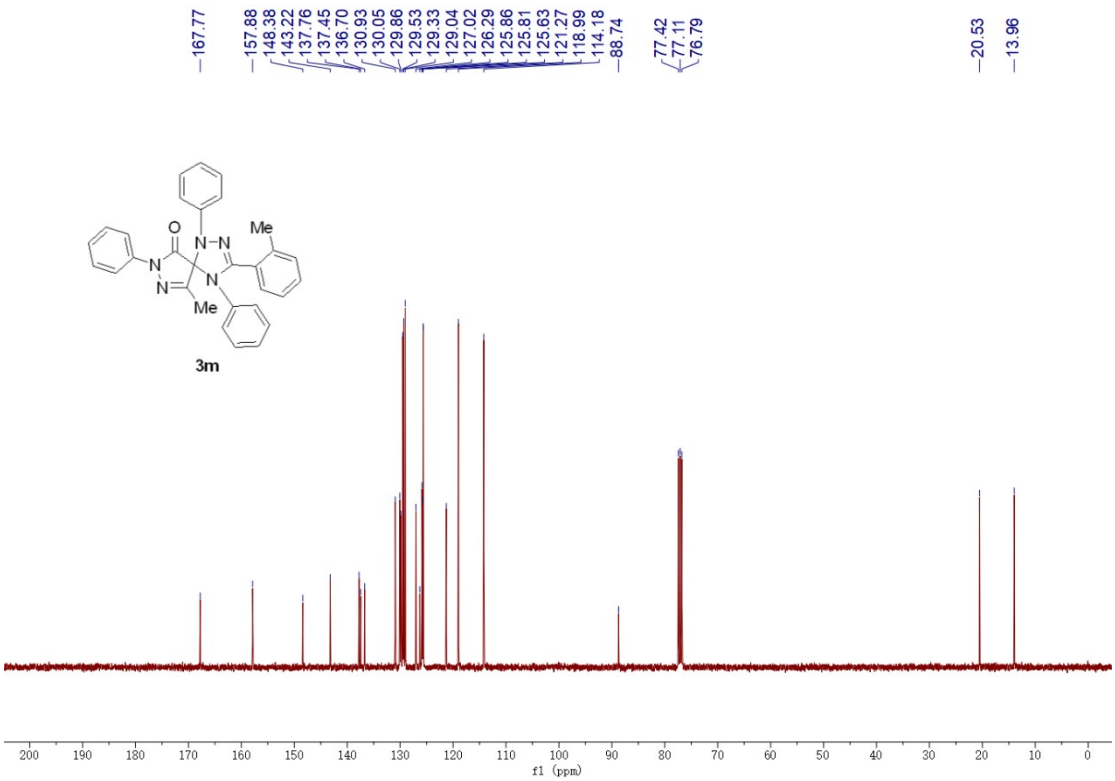
9-methyl-1,4,7-triphenyl-3-(o-tolyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-

one (3m)

^{1}H NMR ($CDCl_3$, 400 MHz)



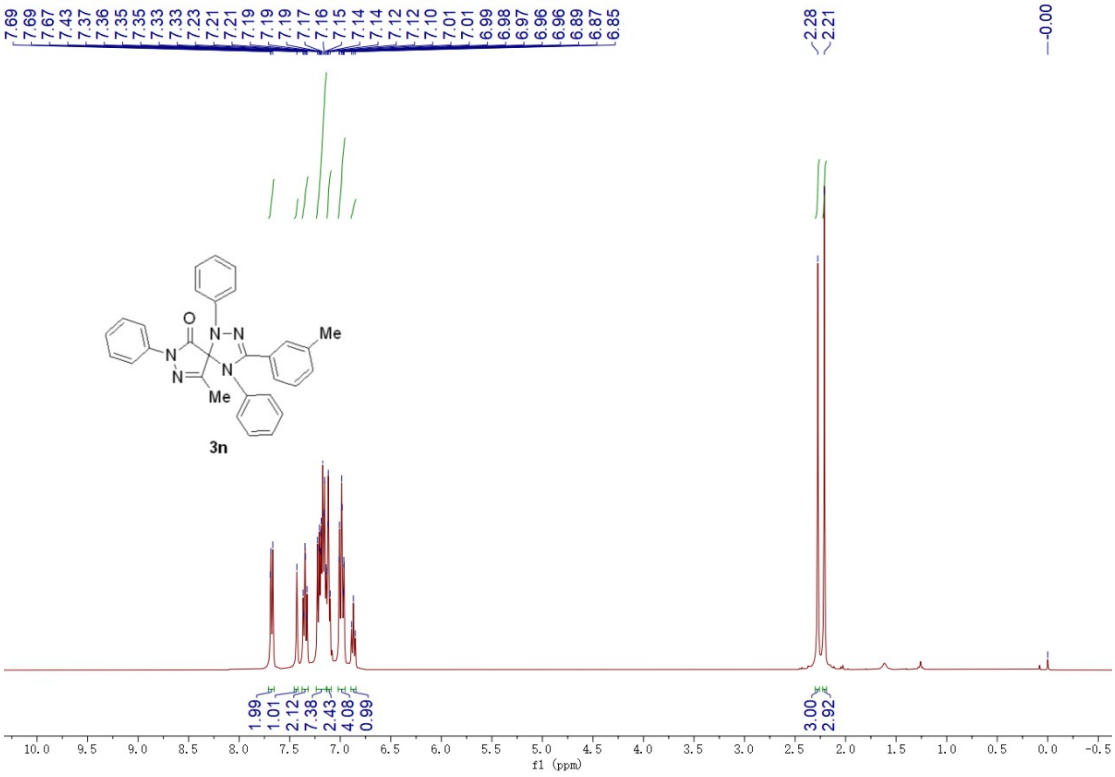
^{13}C NMR ($CDCl_3$, 100 MHz)



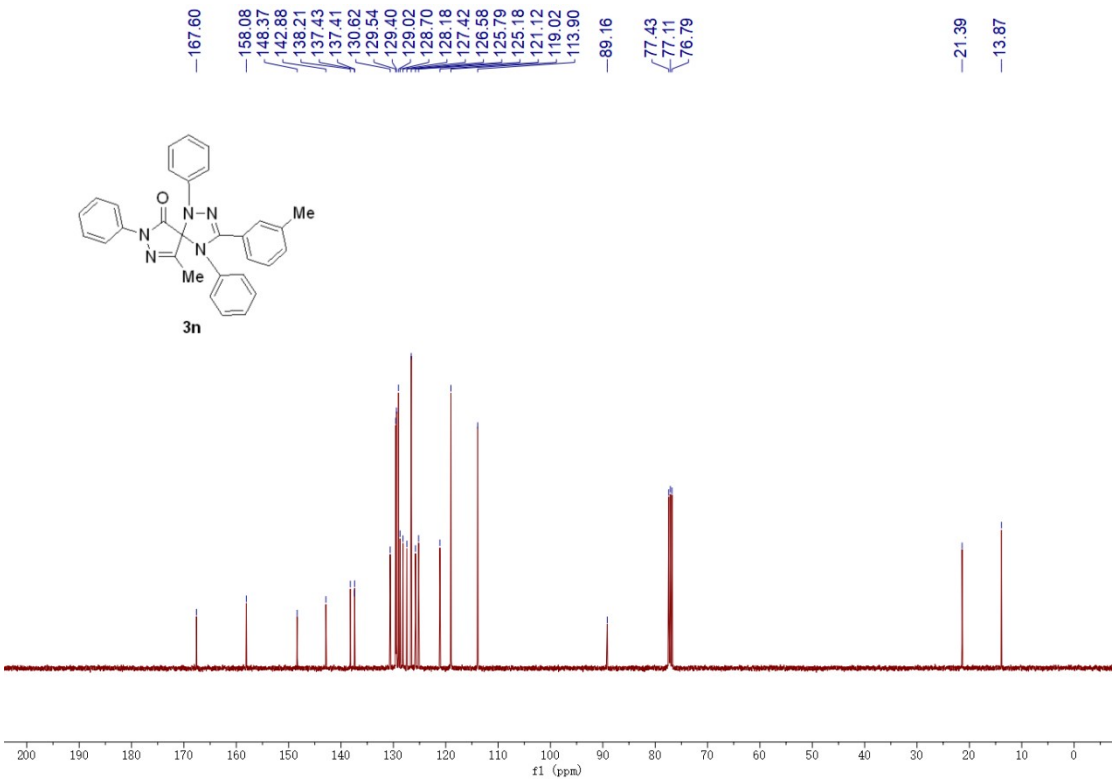
9-methyl-1,4,7-triphenyl-3-(m-tolyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-

one (3n)

^{1}H NMR ($CDCl_3$, 400 MHz)



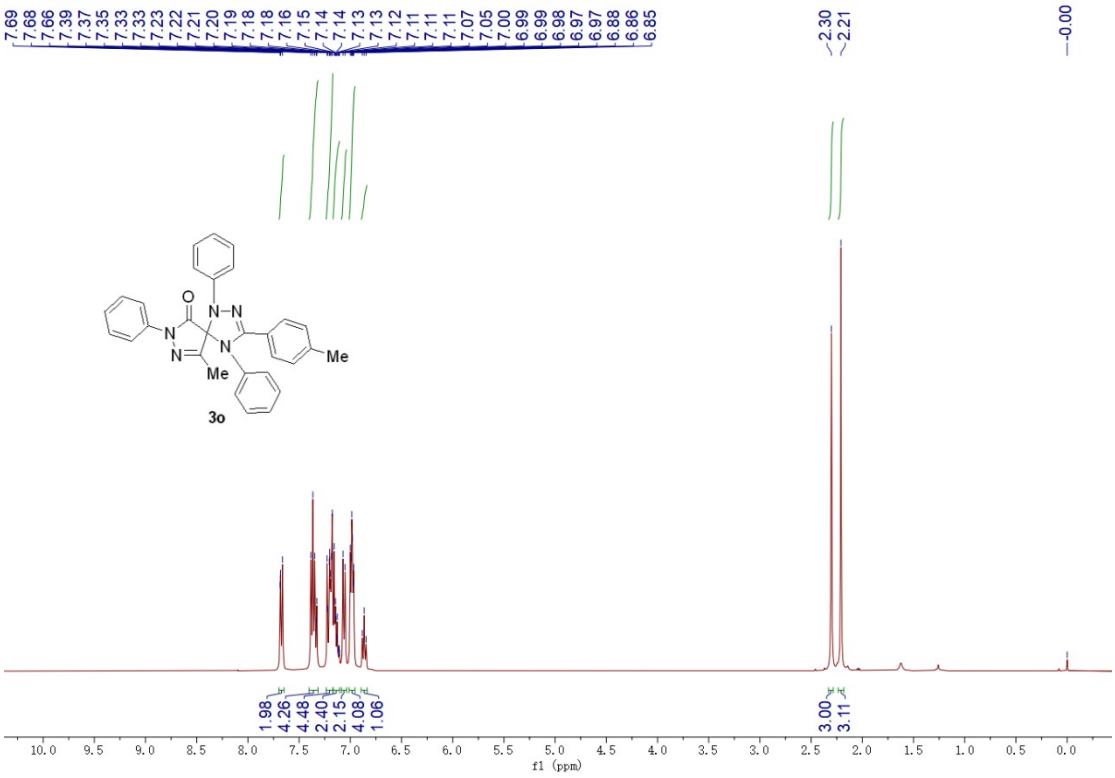
^{13}C NMR ($CDCl_3$, 100 MHz)



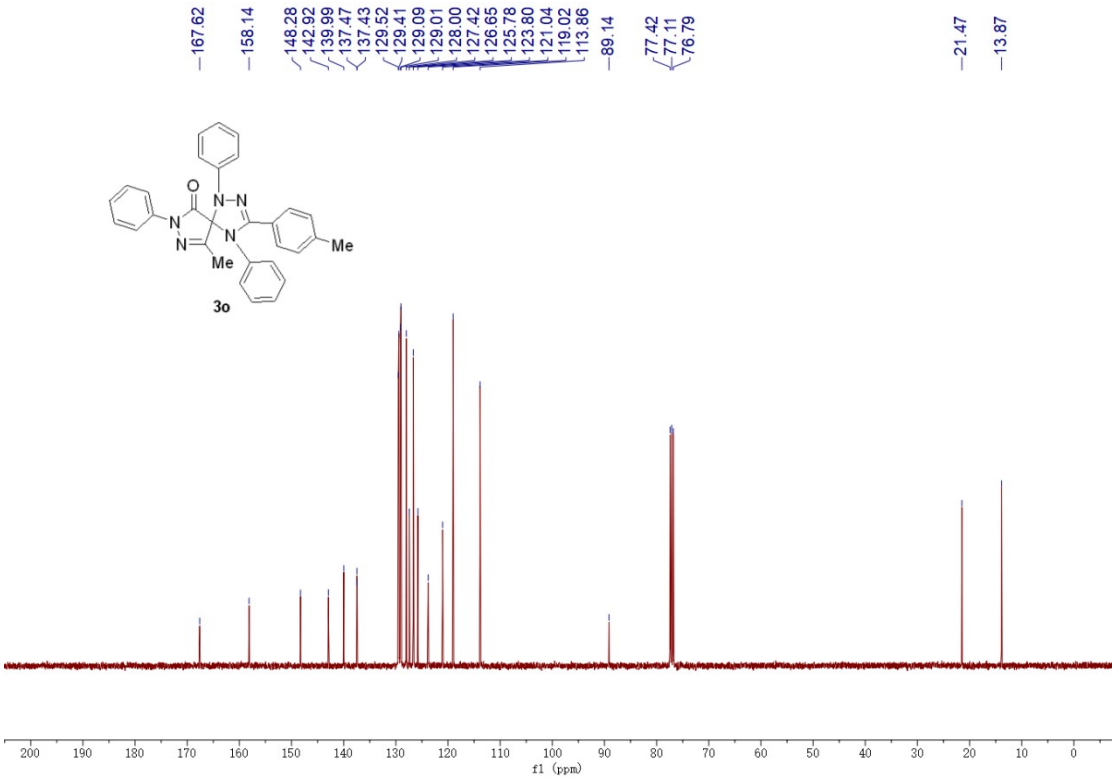
9-methyl-1,4,7-triphenyl-3-(p-tolyl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-

one (3o)

^{1}H NMR ($CDCl_3$, 400 MHz)



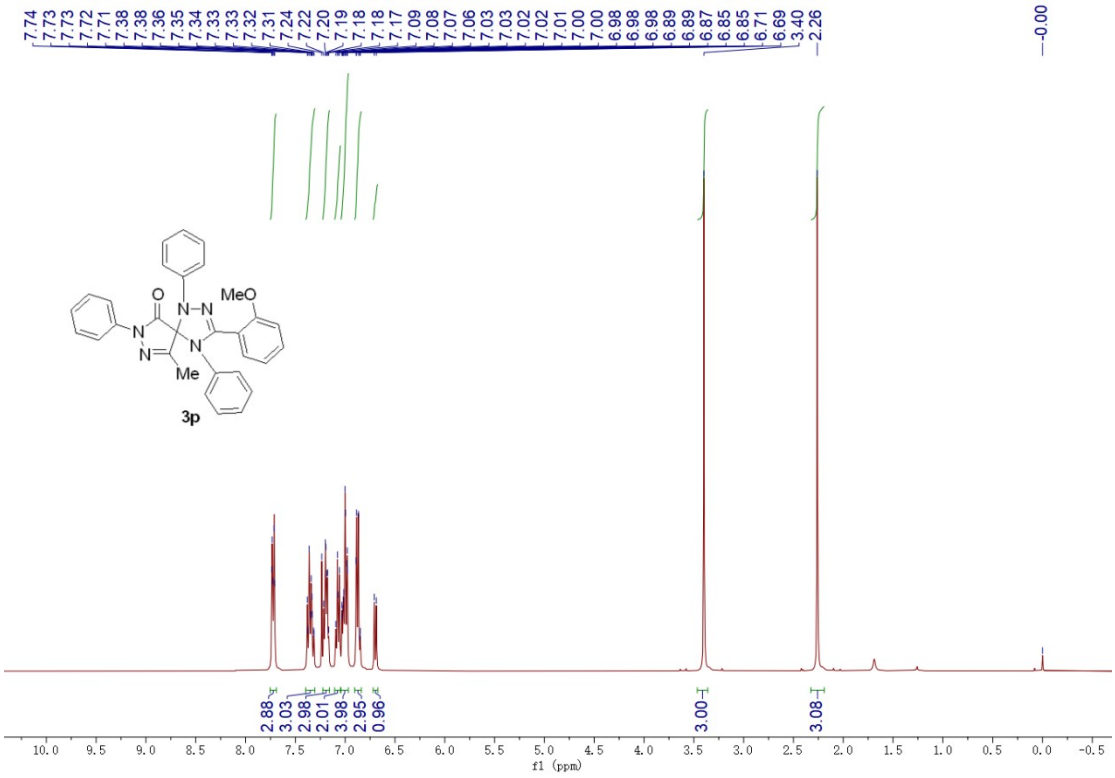
^{13}C NMR ($CDCl_3$, 100 MHz)



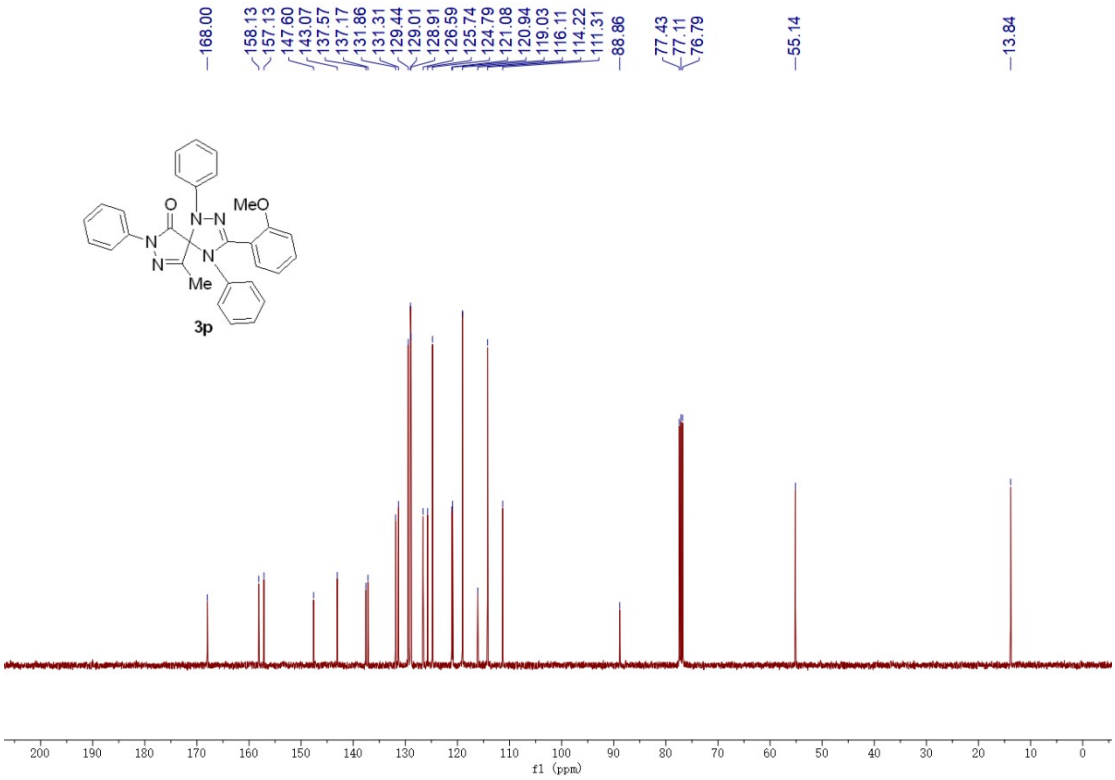
3-(2-methoxyphenyl)-9-methyl-1,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3p)

^{1}H NMR ($CDCl_3$, 400 MHz)



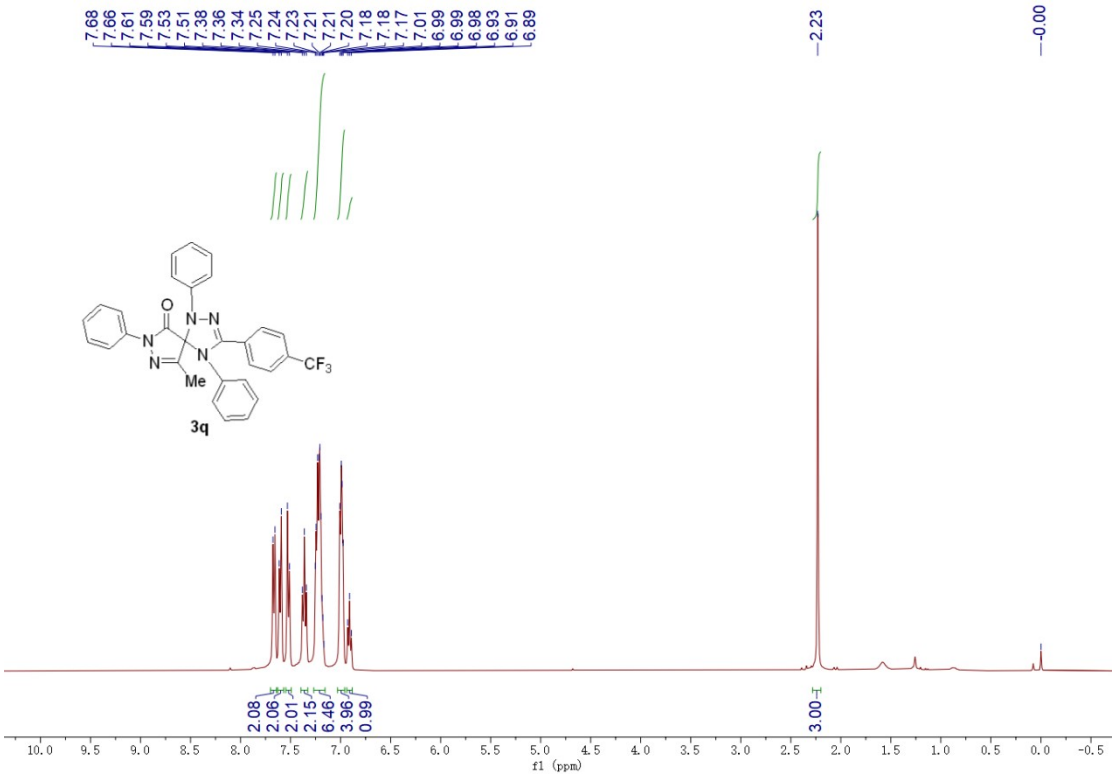
^{13}C NMR ($CDCl_3$, 100 MHz)



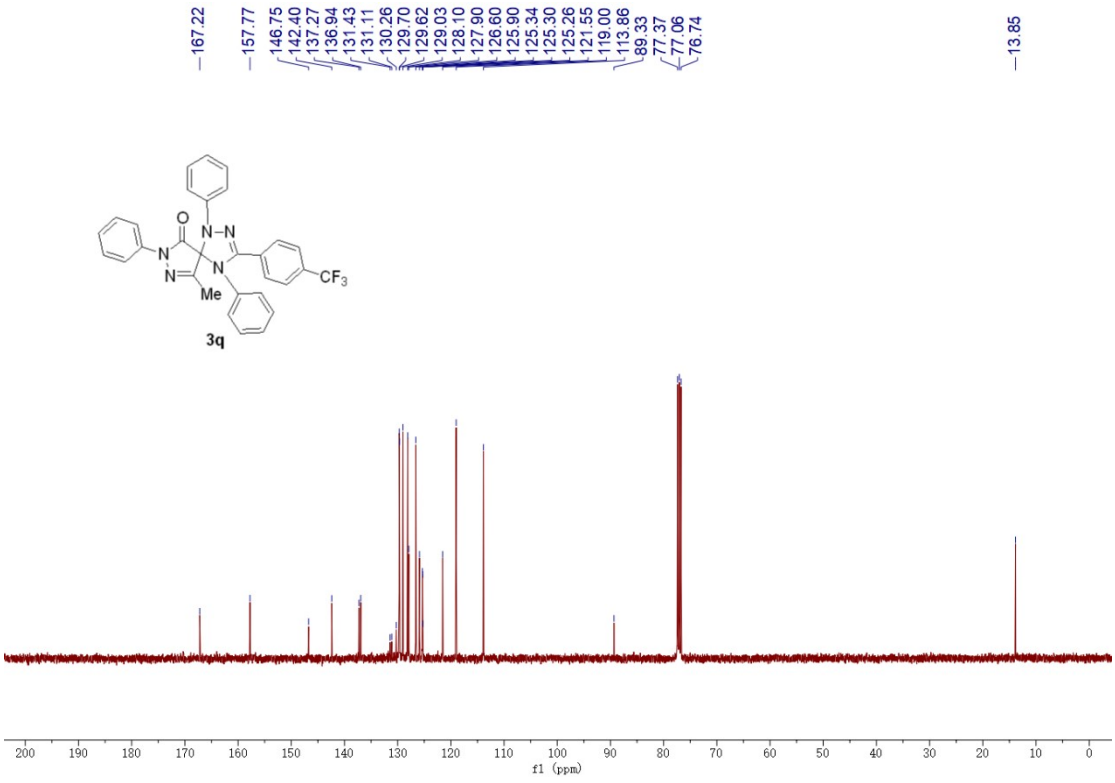
9-methyl-1,4,7-triphenyl-3-(4-(trifluoromethyl)phenyl)-1,2,4,7,8-

pentaazaspiro[4.4]nona-2,8-dien-6-one (3q)

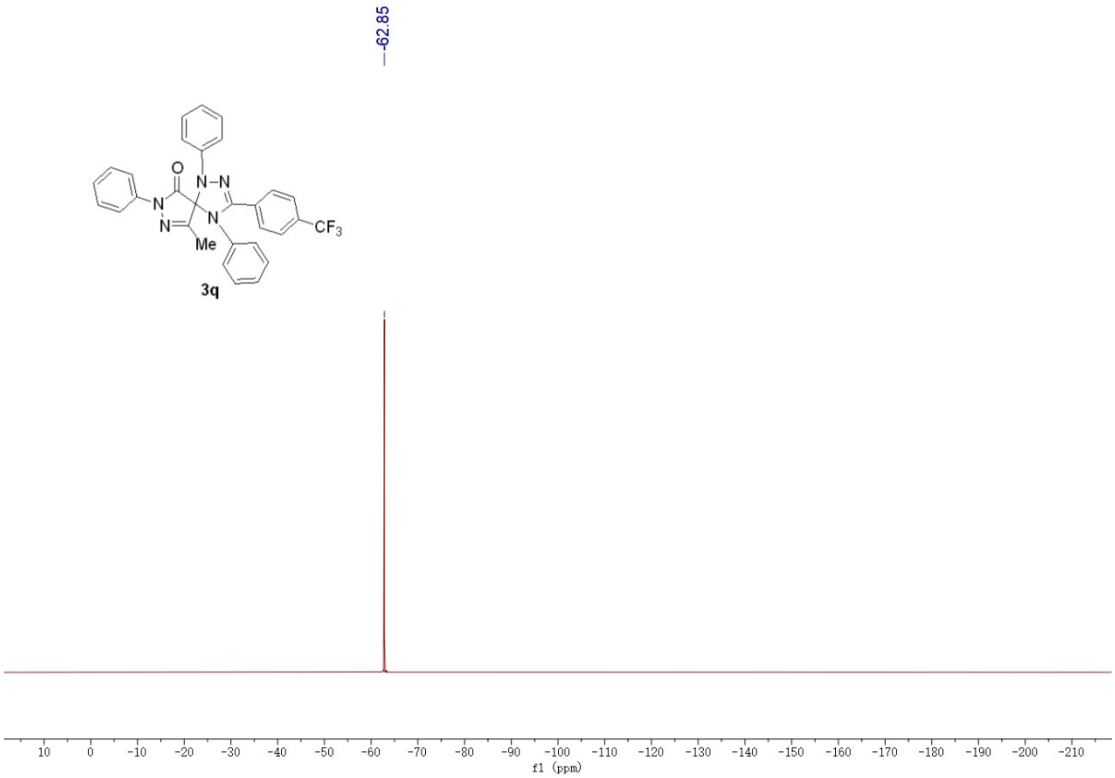
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



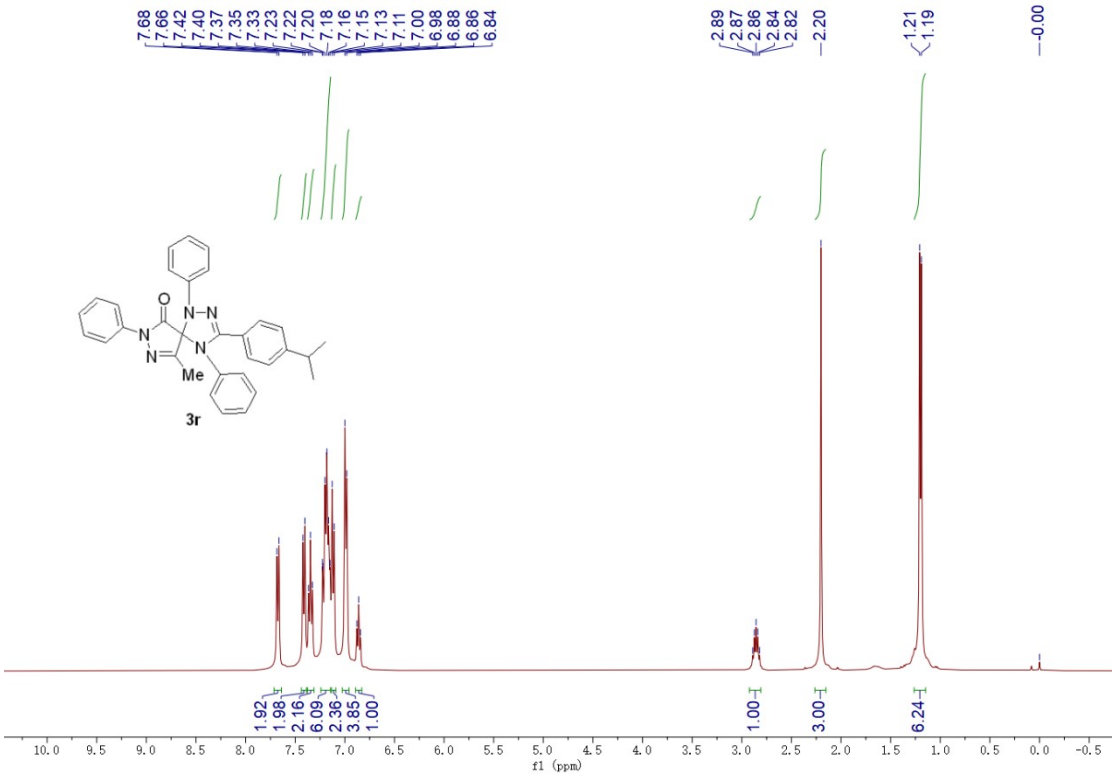
^{19}F NMR ($CDCl_3$, 376 MHz)



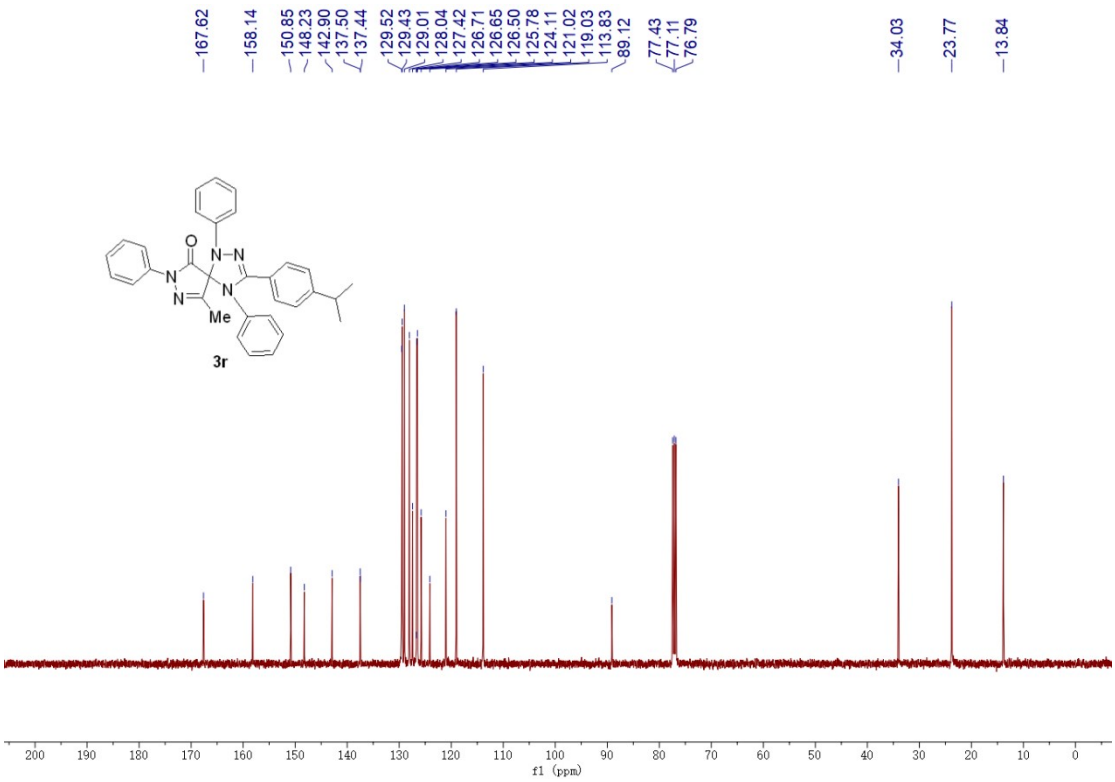
3-(4-isopropylphenyl)-9-methyl-1,4,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3r)

^{1}H NMR ($CDCl_3$, 400 MHz)



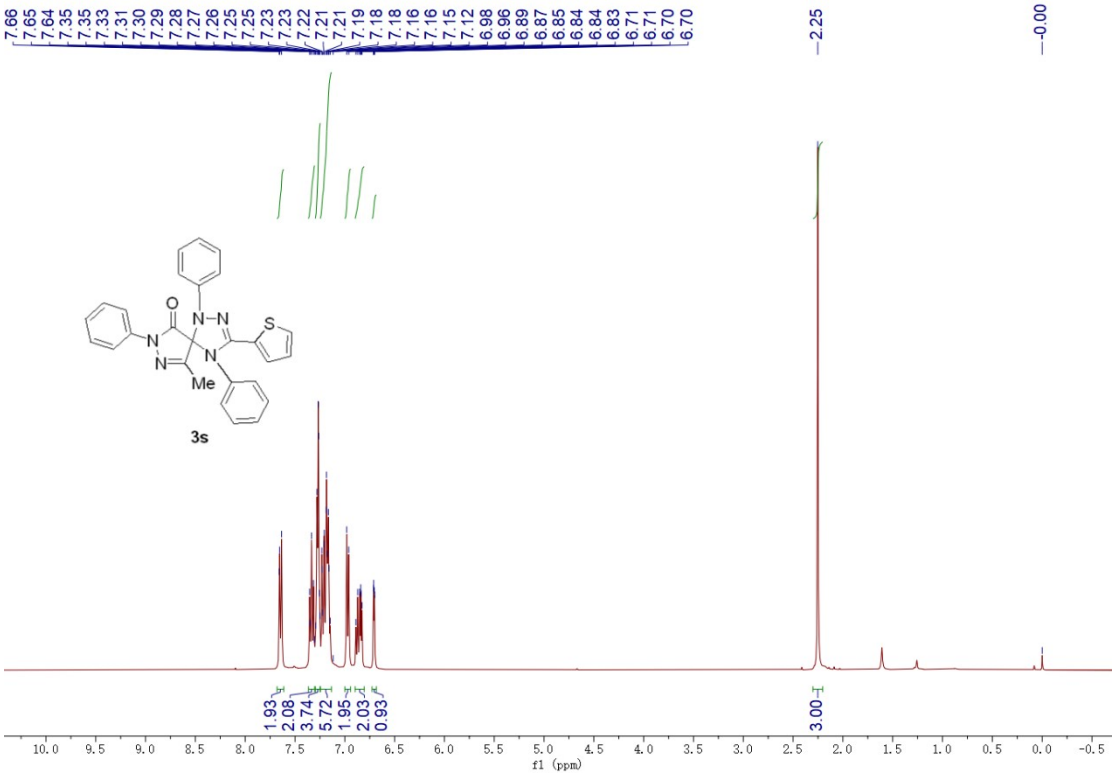
^{13}C NMR ($CDCl_3$, 100 MHz)



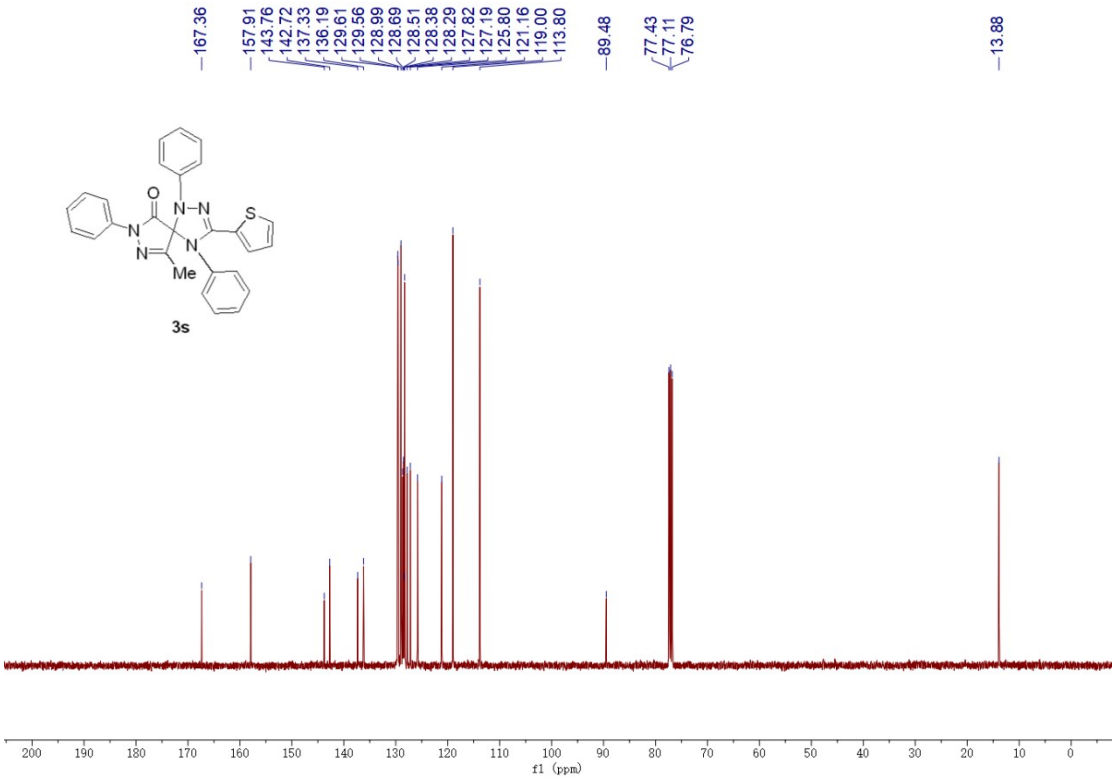
9-methyl-1,4,7-triphenyl-3-(thiophen-2-yl)-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-

dien-6-one (3s)

^{1}H NMR ($CDCl_3$, 400 MHz)



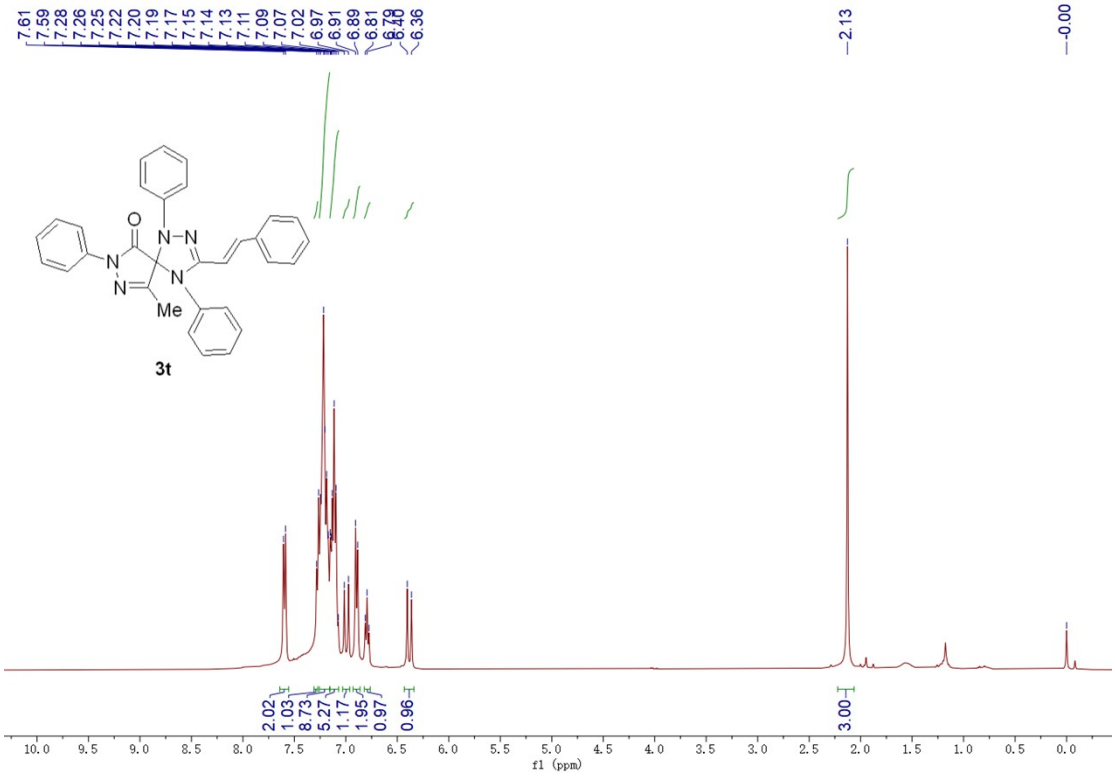
^{13}C NMR ($CDCl_3$, 100 MHz)



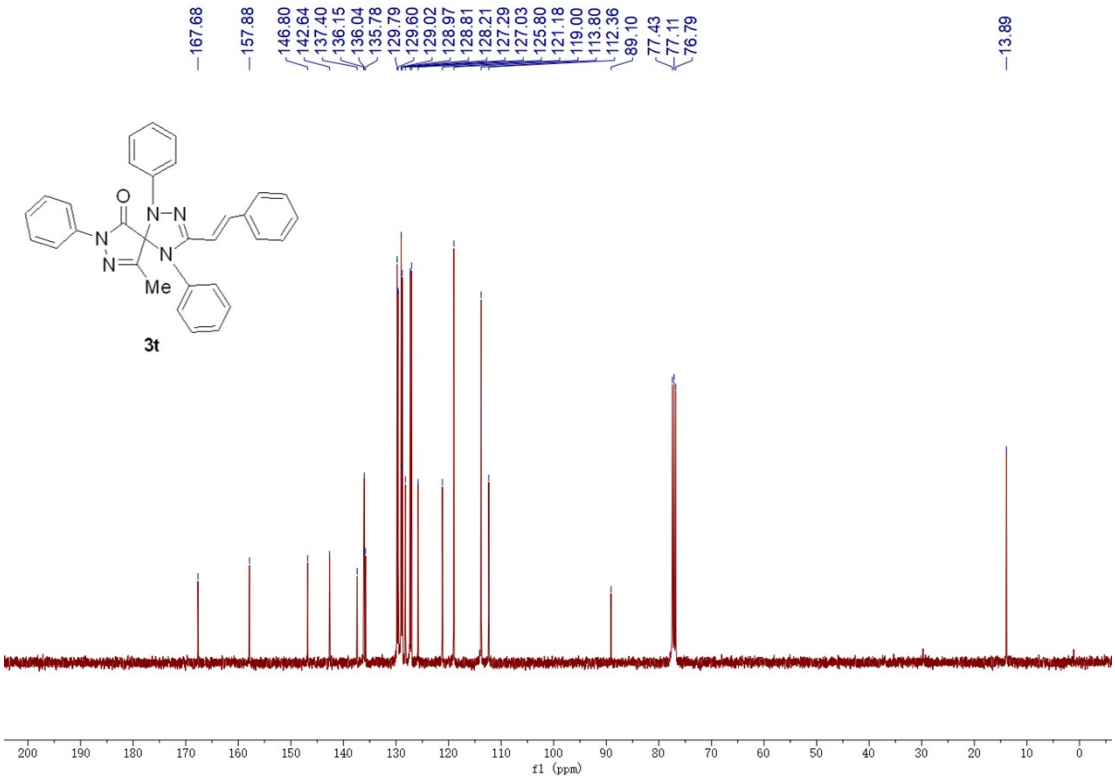
9-methyl-1,4,7-triphenyl-3-styryl-1,2,4,7,8-pentaazaspiro[4.4]nona-2,8-dien-6-one

(3t)

^{1}H NMR ($CDCl_3$, 400 MHz)



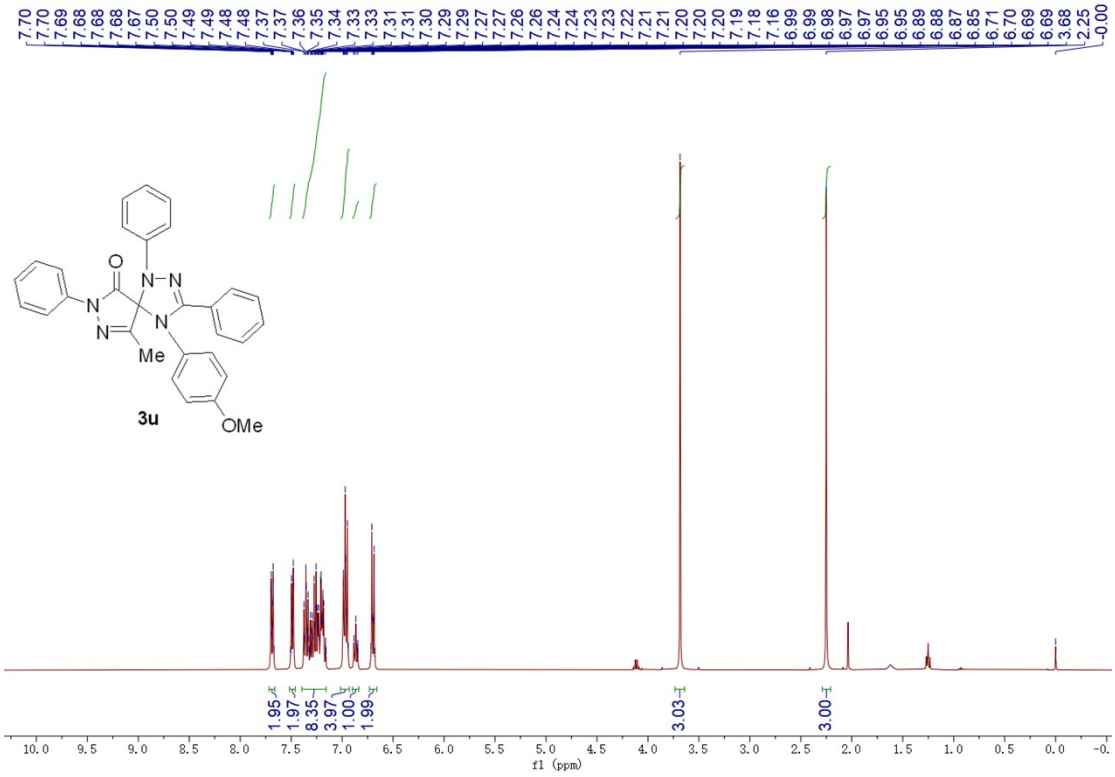
^{13}C NMR ($CDCl_3$, 100 MHz)



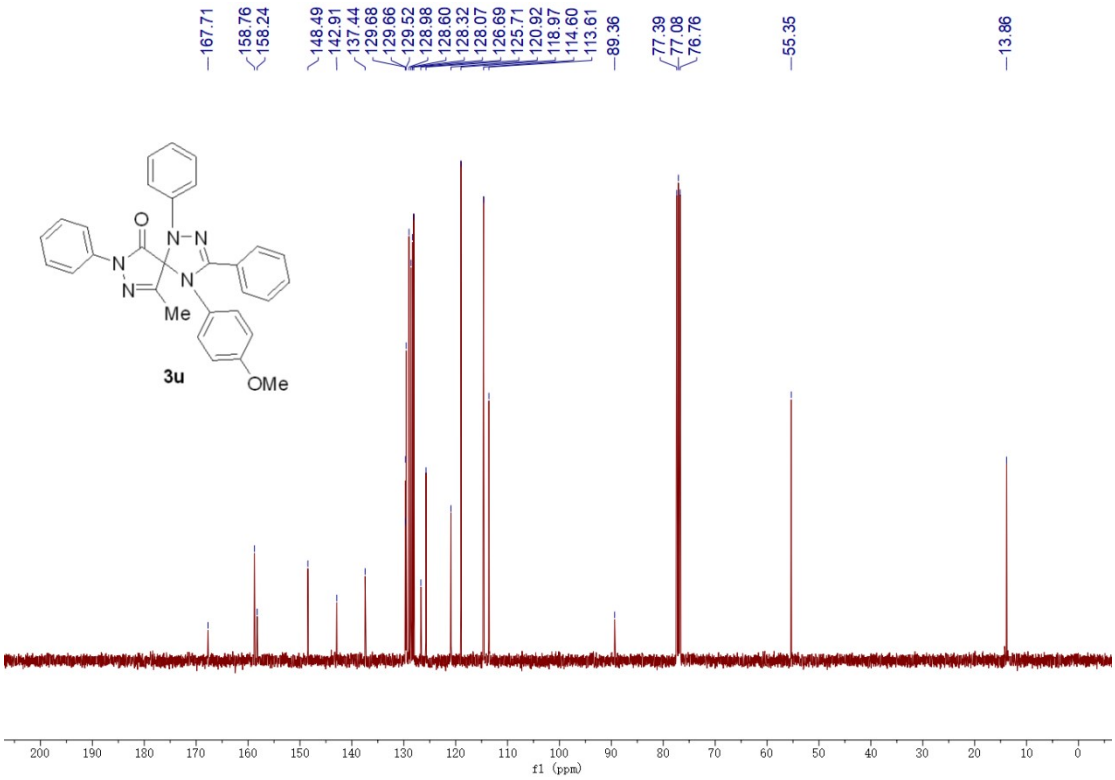
4-(4-methoxyphenyl)-9-methyl-1,3,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3u)

^{1}H NMR ($CDCl_3$, 400 MHz)



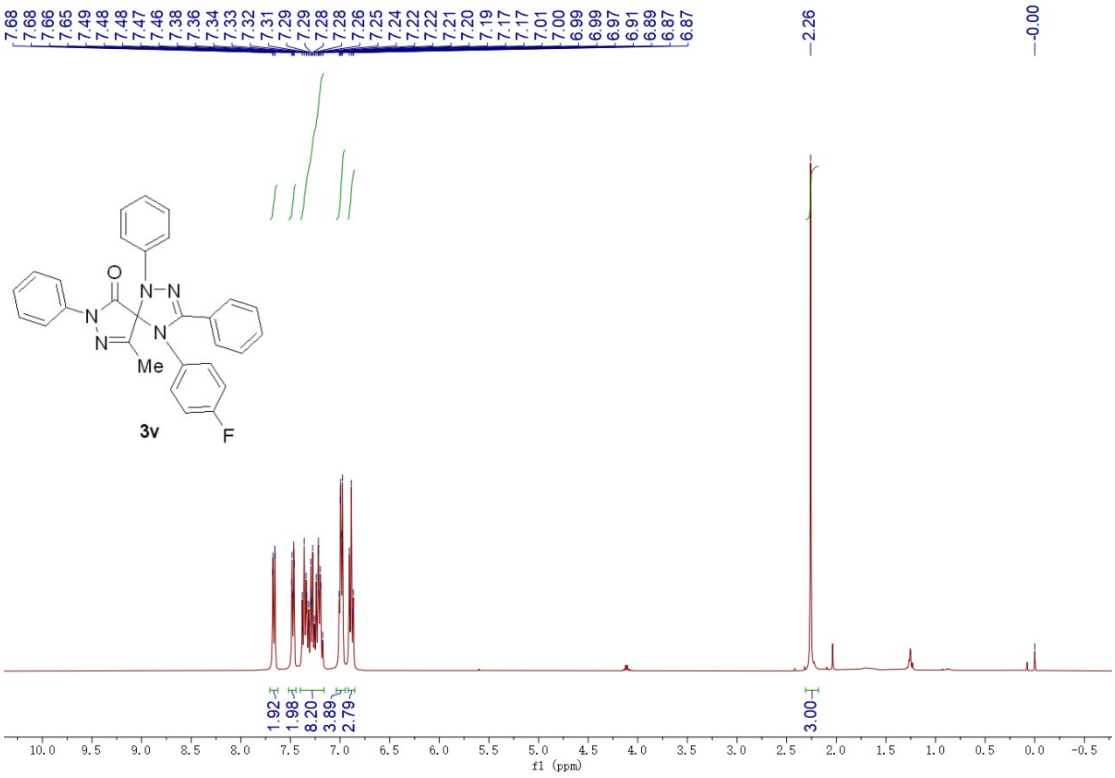
^{13}C NMR ($CDCl_3$, 100 MHz)



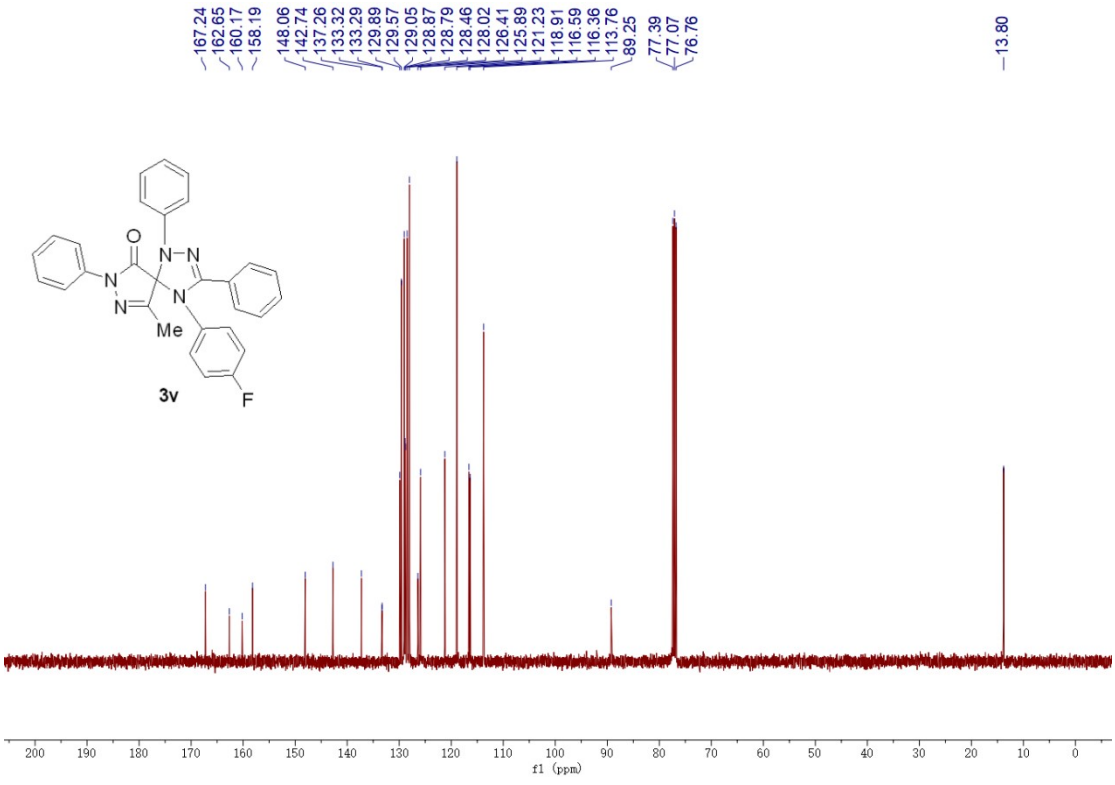
4-(4-fluorophenyl)-9-methyl-1,3,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3v)

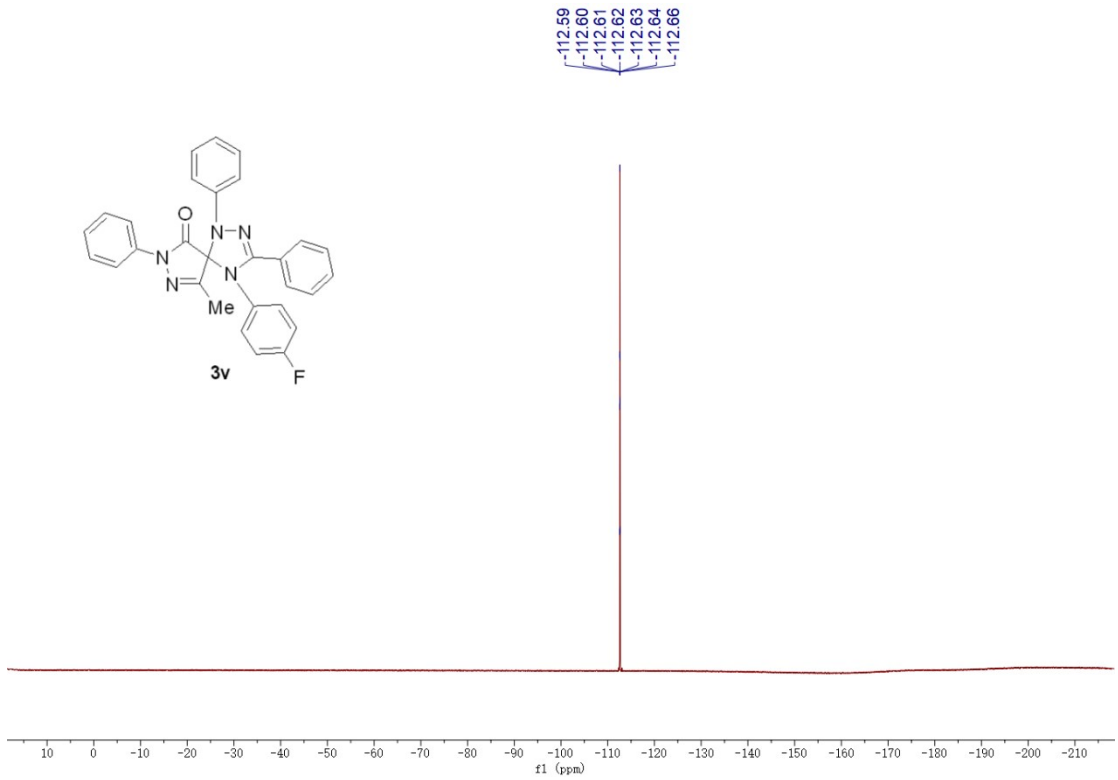
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



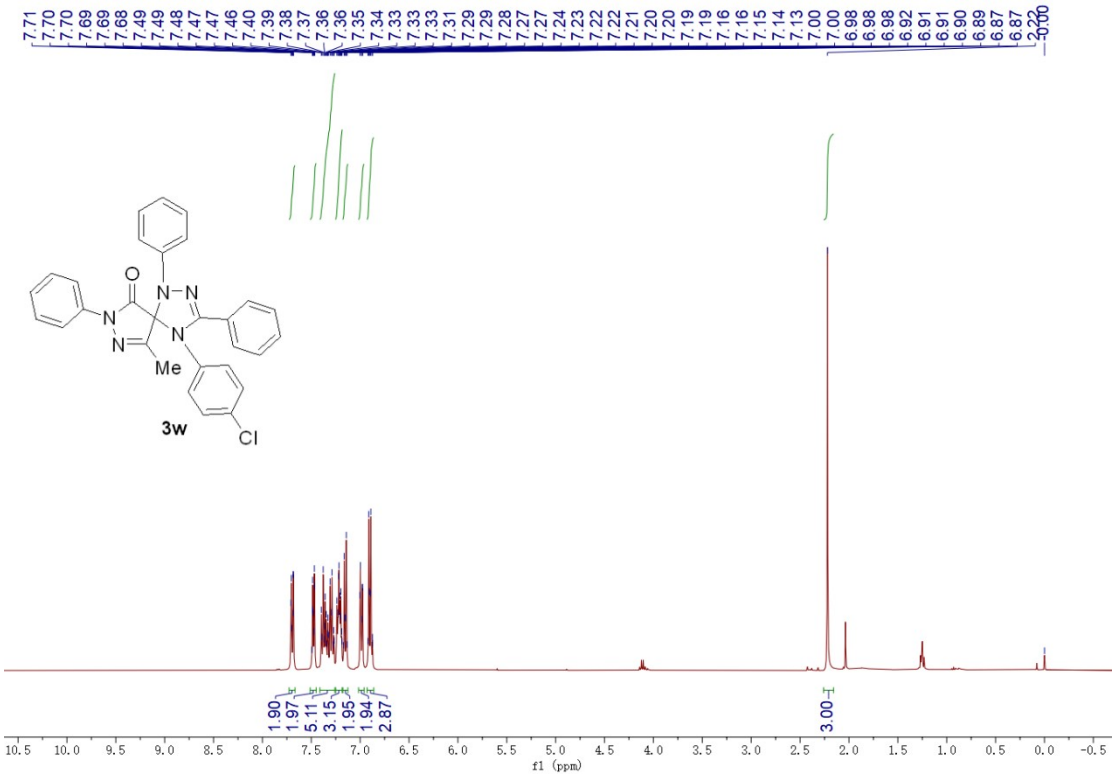
^{19}F NMR ($CDCl_3$, 376 MHz)



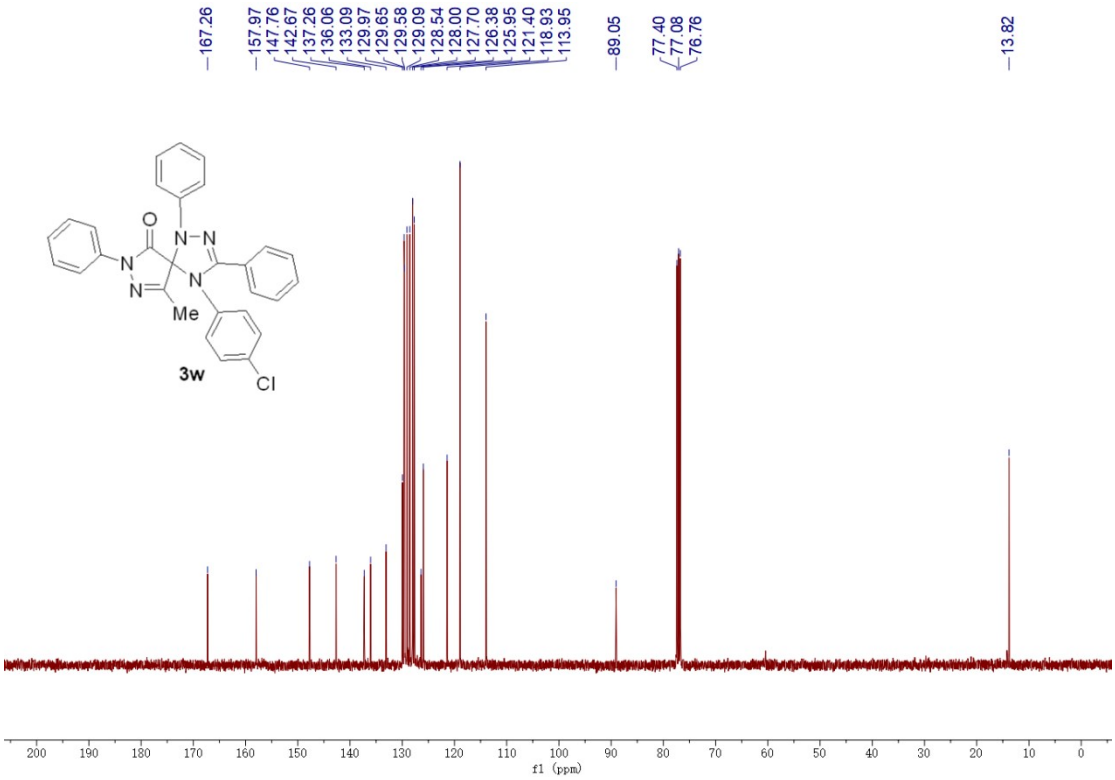
4-(4-chlorophenyl)-9-methyl-1,3,7-triphenyl-1,2,4,7,8-pentaazaspiro[4.4]nona-

2,8-dien-6-one (3w)

^{1}H NMR ($CDCl_3$, 400 MHz)



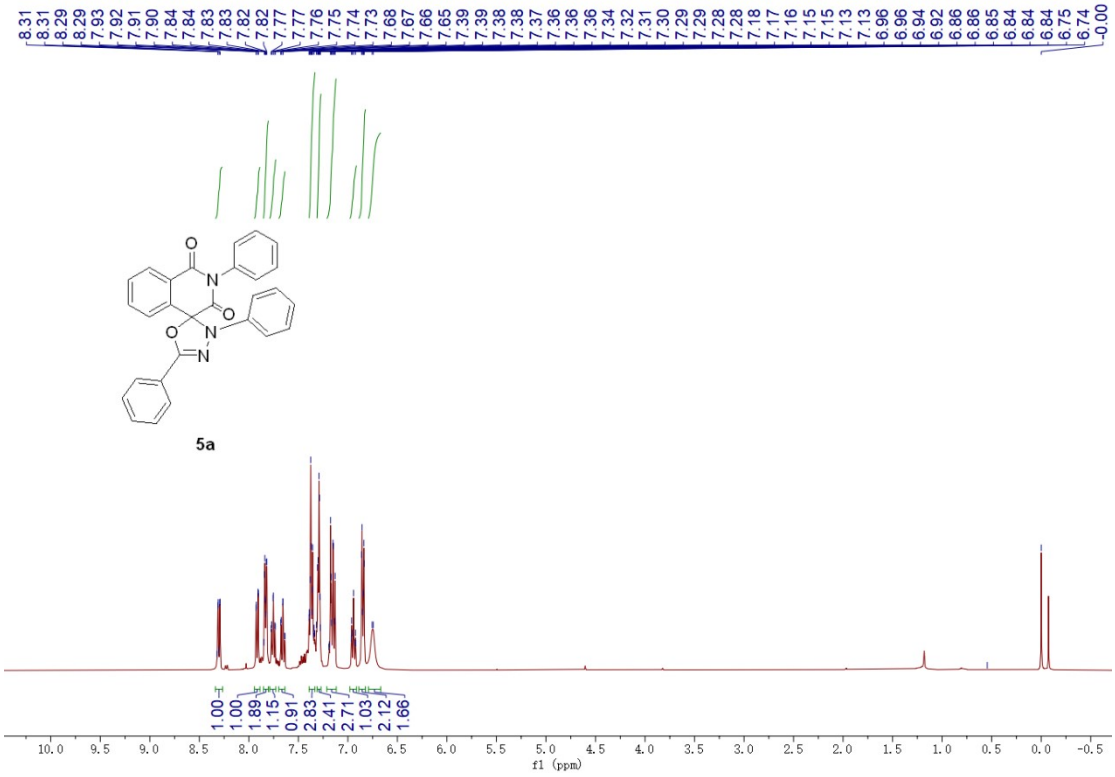
^{13}C NMR ($CDCl_3$, 100 MHz)



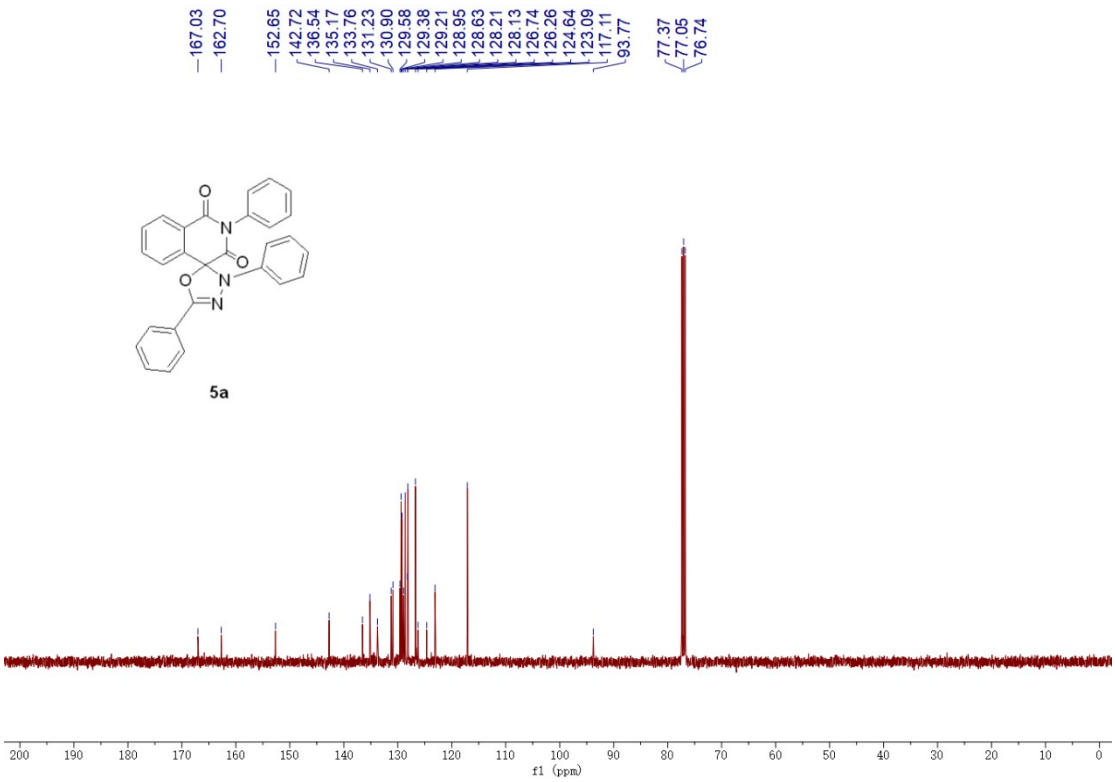
2,3',5'-triphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2*H*)-dione

(5a)

^{1}H NMR ($CDCl_3$, 400 MHz)



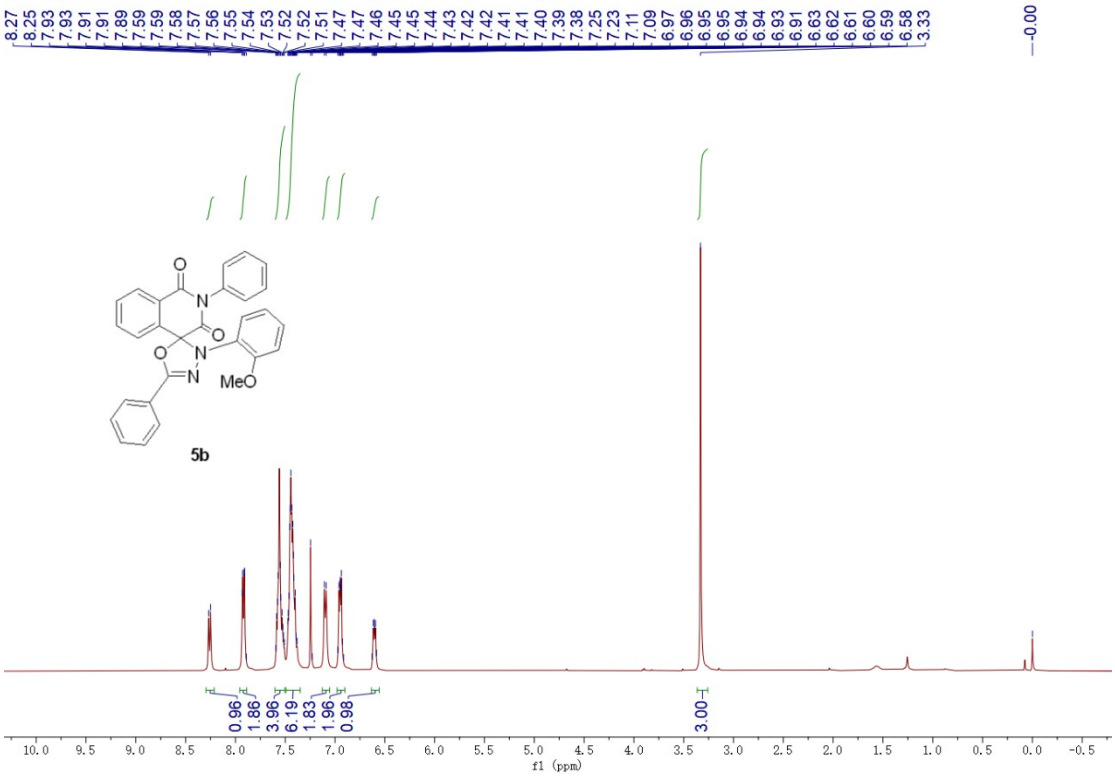
^{13}C NMR ($CDCl_3$, 100 MHz)



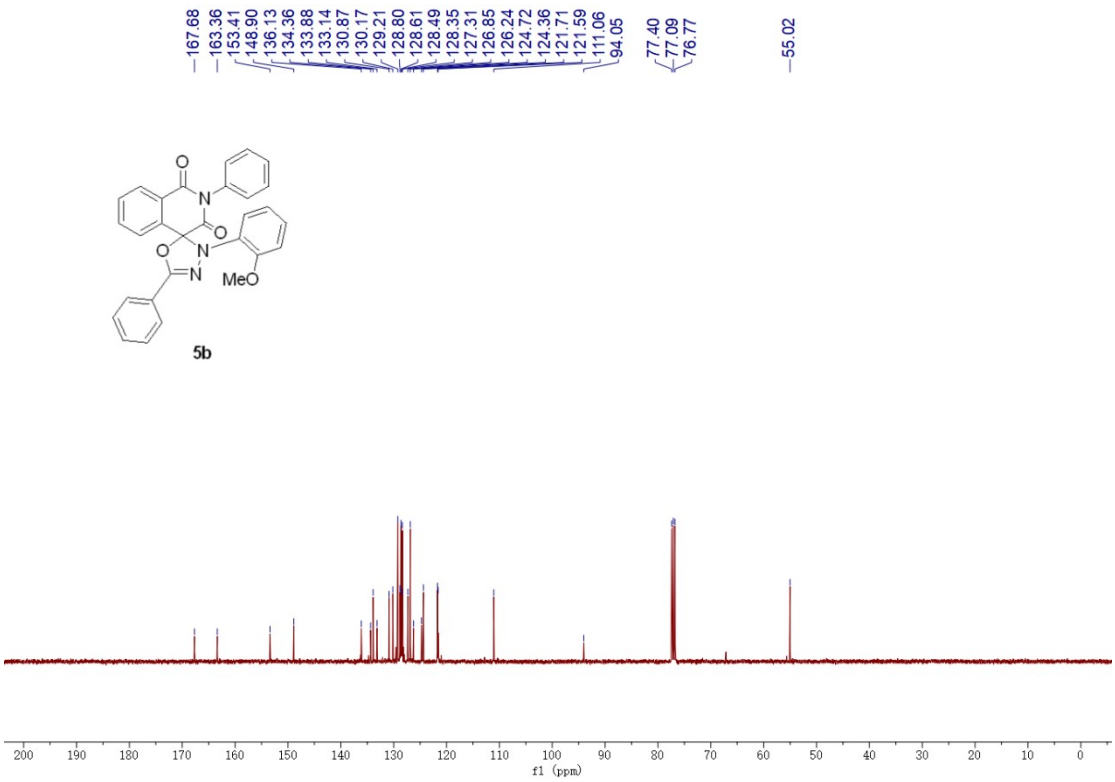
3'-(2-methoxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5b)

^{1}H NMR ($CDCl_3$, 400 MHz)



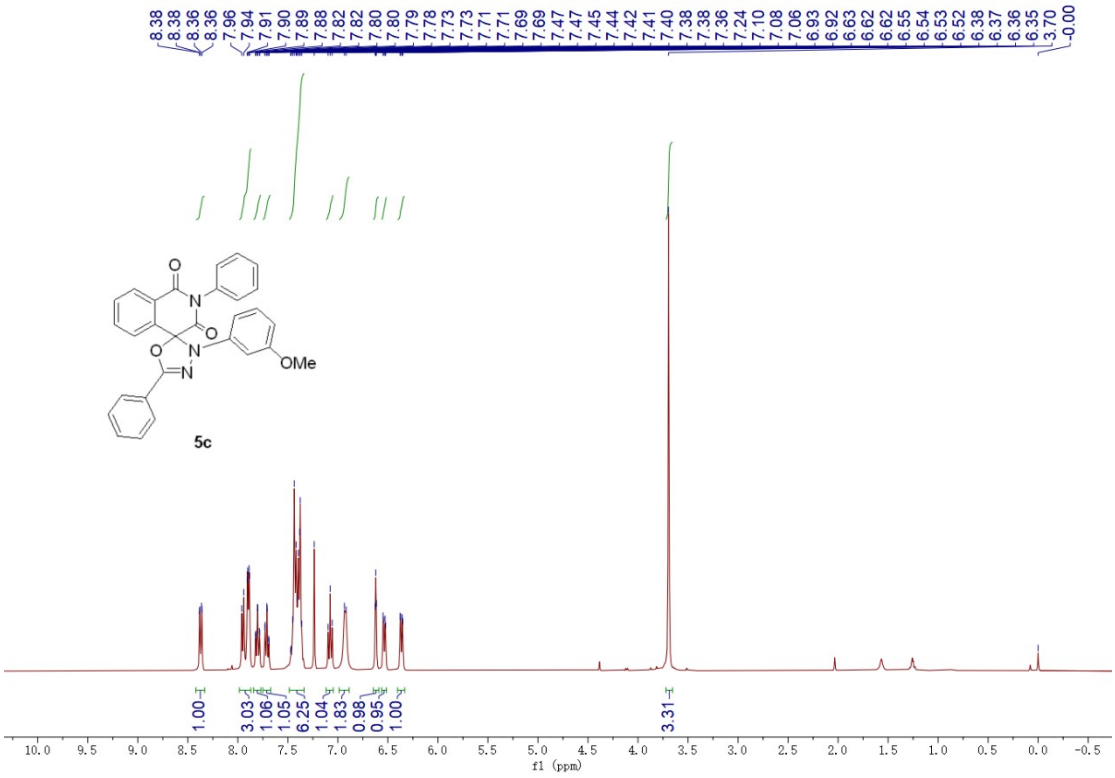
^{13}C NMR ($CDCl_3$, 100 MHz)



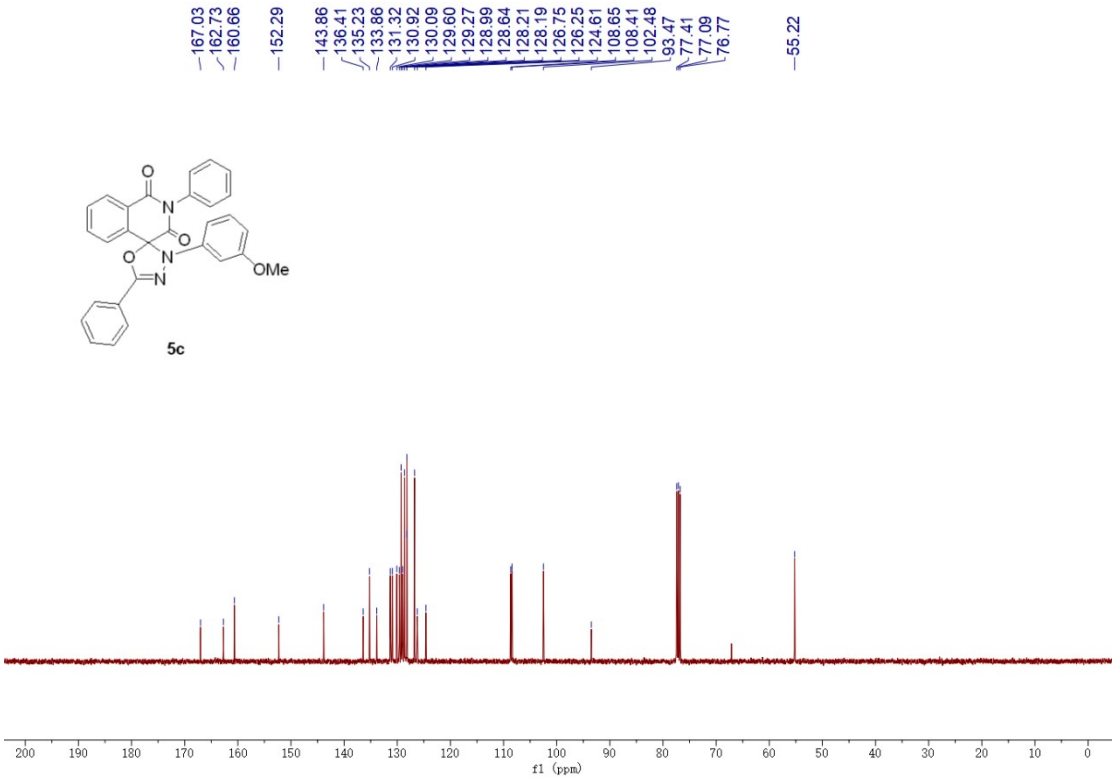
3'-(3-methoxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5c)

^{1}H NMR ($CDCl_3$, 400 MHz)



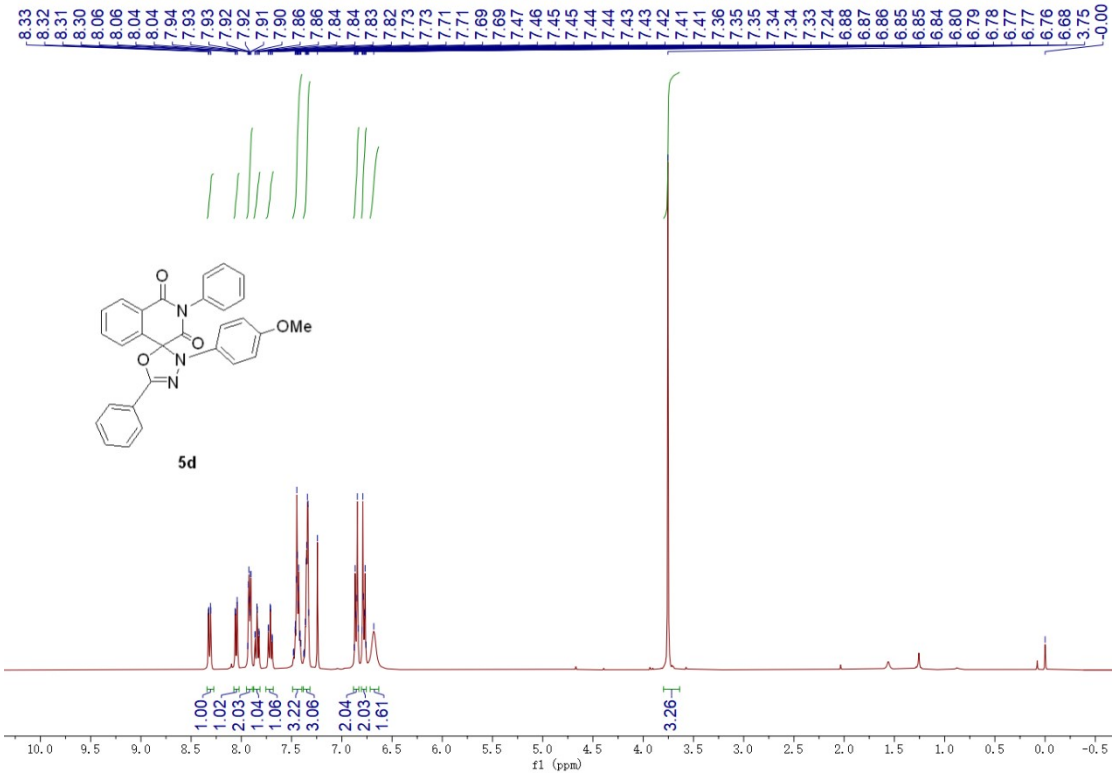
^{13}C NMR ($CDCl_3$, 100 MHz)



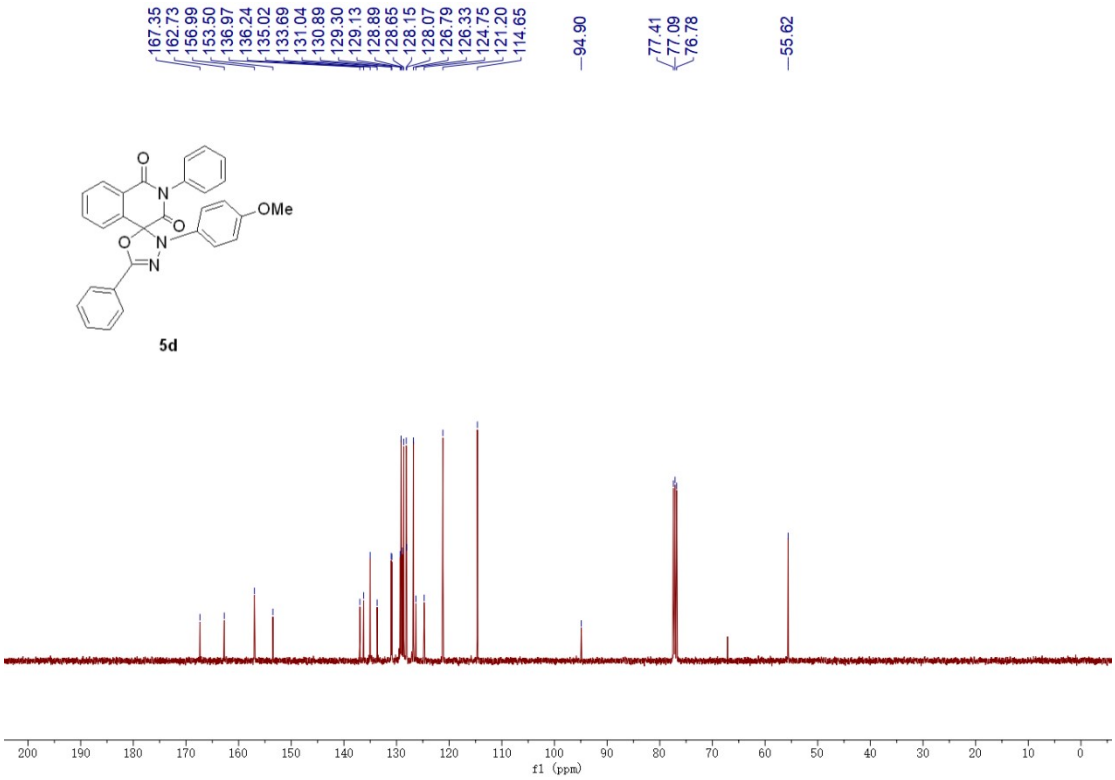
3'-(4-methoxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5d)

^{1}H NMR ($CDCl_3$, 400 MHz)



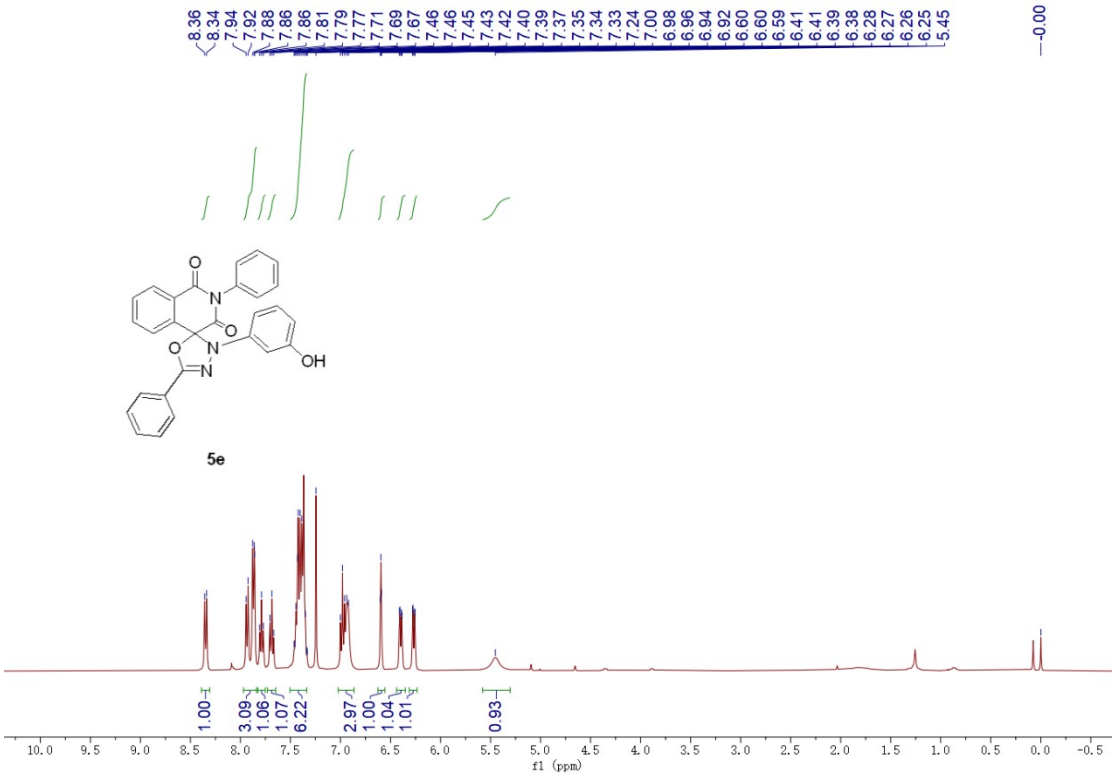
^{13}C NMR ($CDCl_3$, 100 MHz)



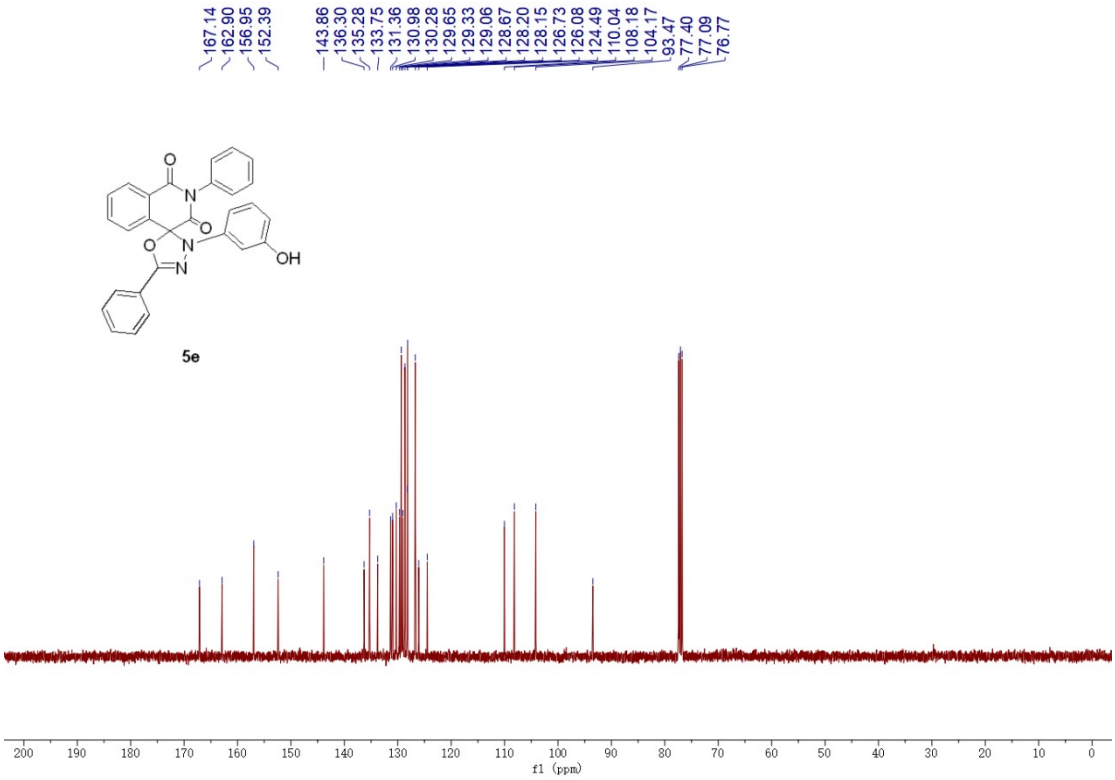
3'-(3-hydroxyphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5e)

^{1}H NMR ($CDCl_3$, 400 MHz)



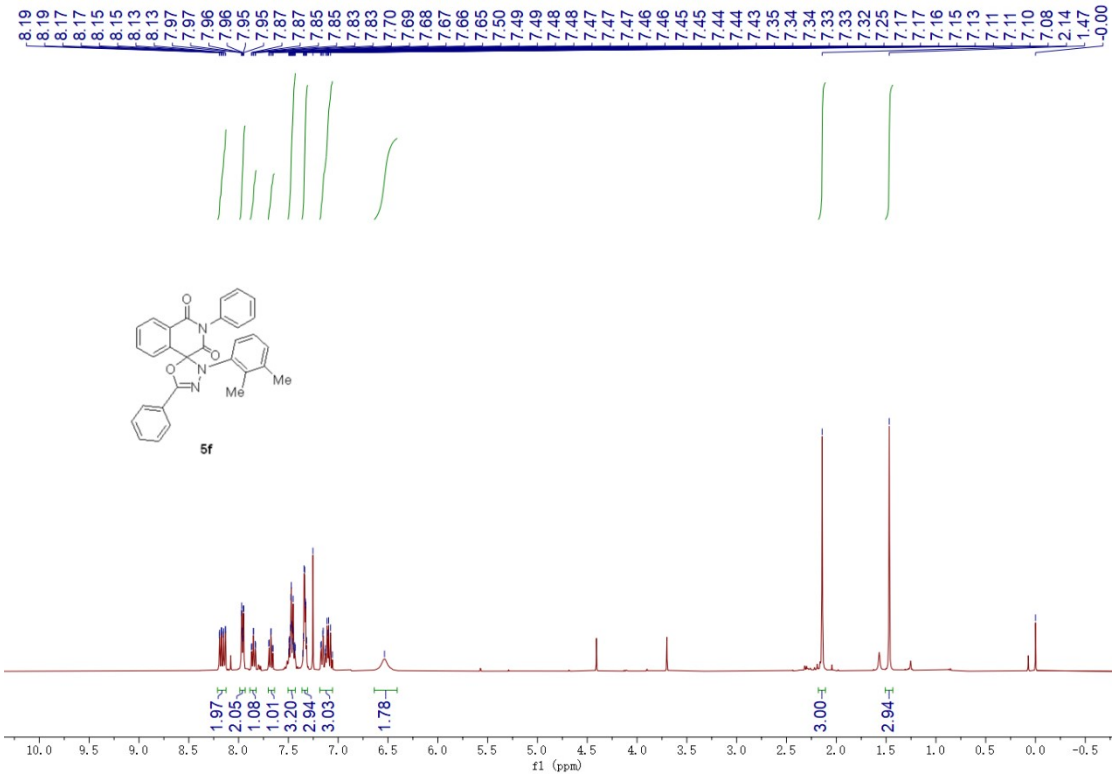
^{13}C NMR ($CDCl_3$, 100 MHz)



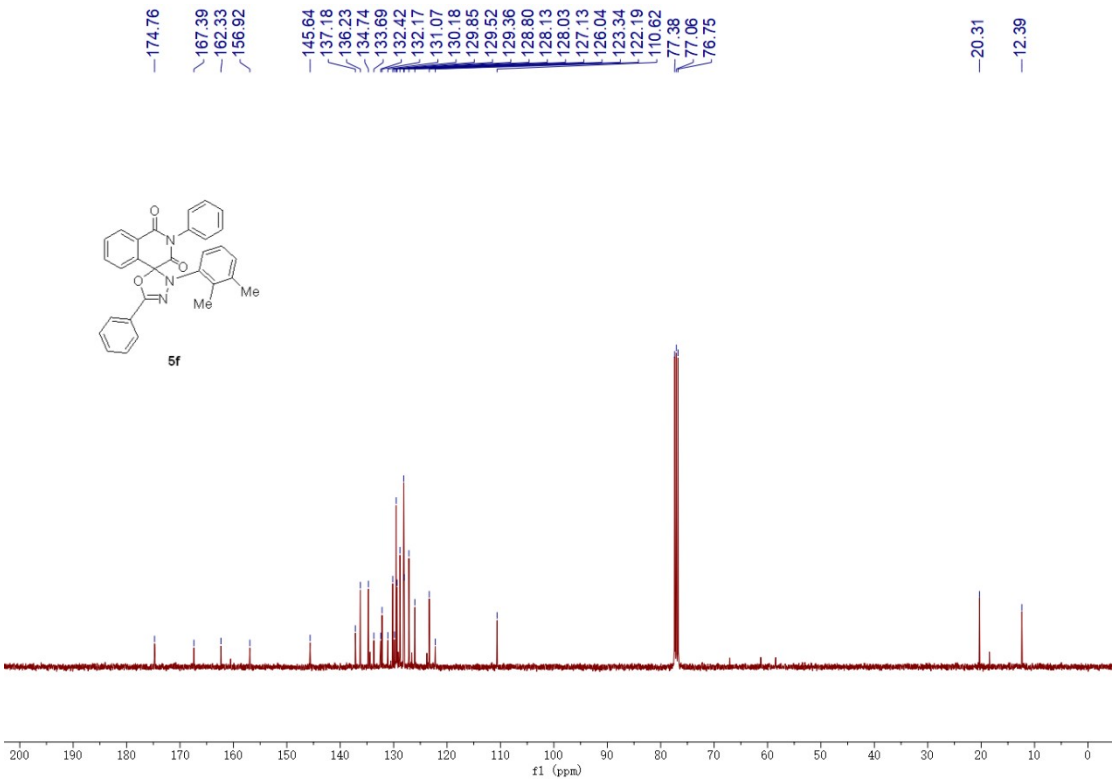
3'-(2,3-dimethylphenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5f)

^{1}H NMR ($CDCl_3$, 400 MHz)



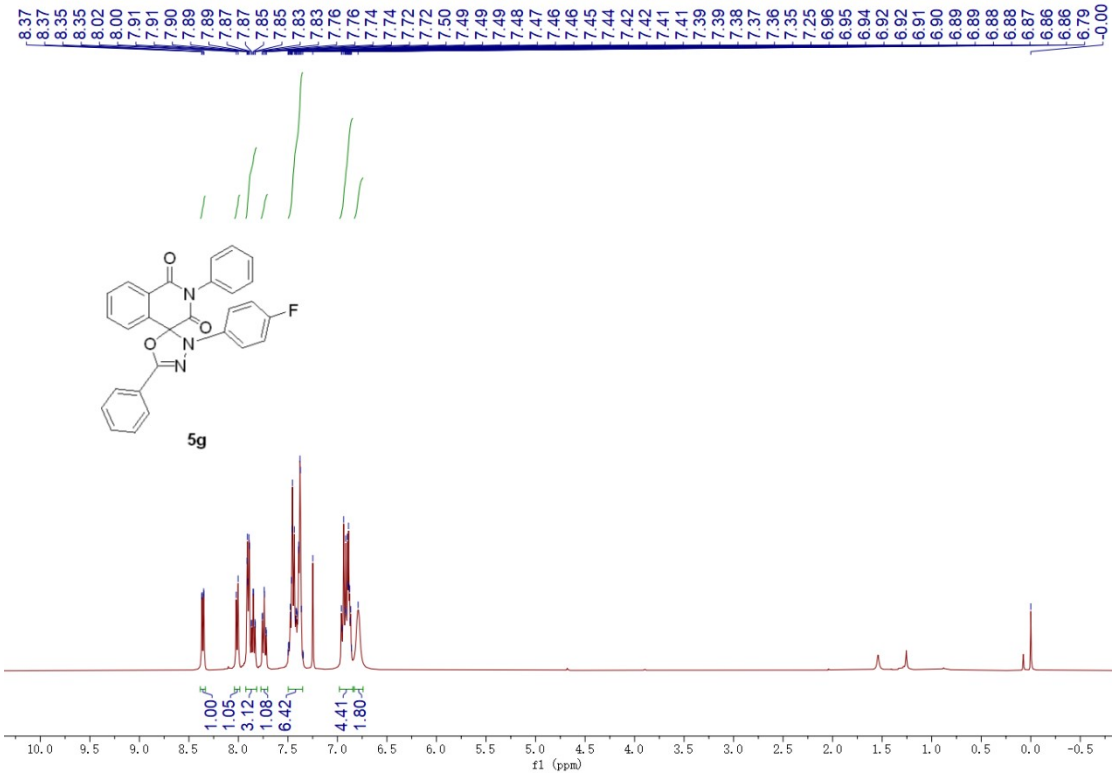
^{13}C NMR ($CDCl_3$, 100 MHz)



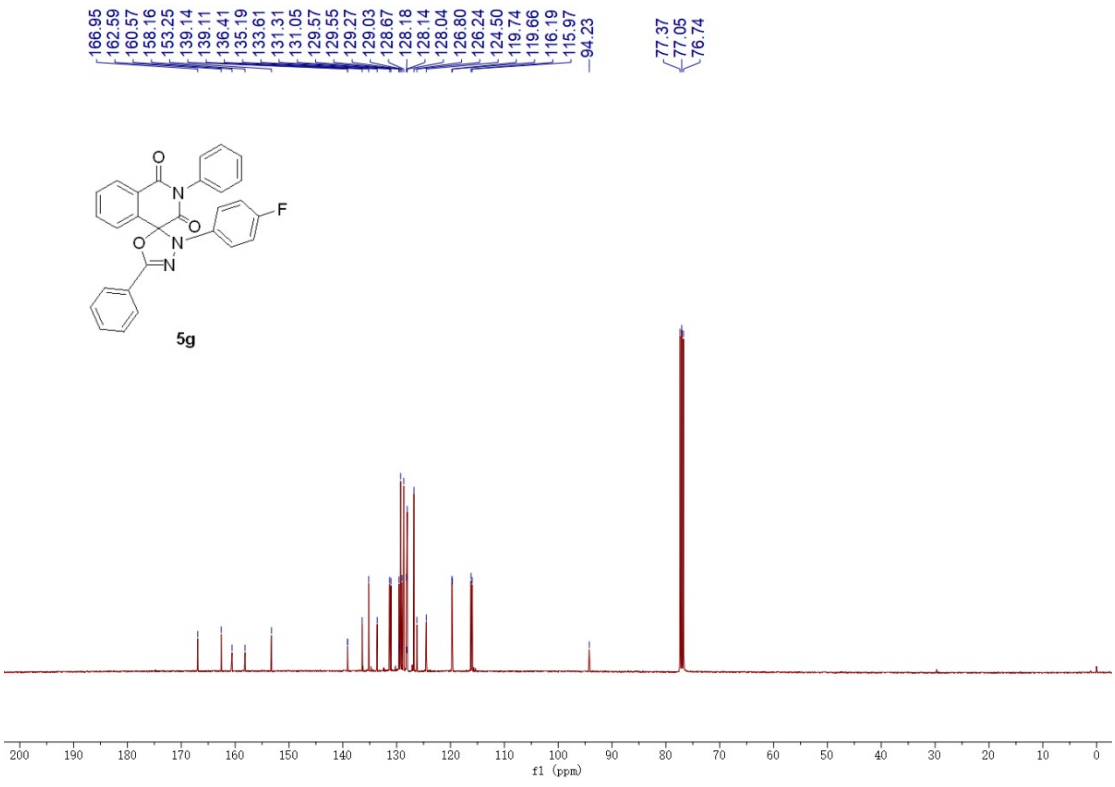
3'-(4-fluorophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5g)

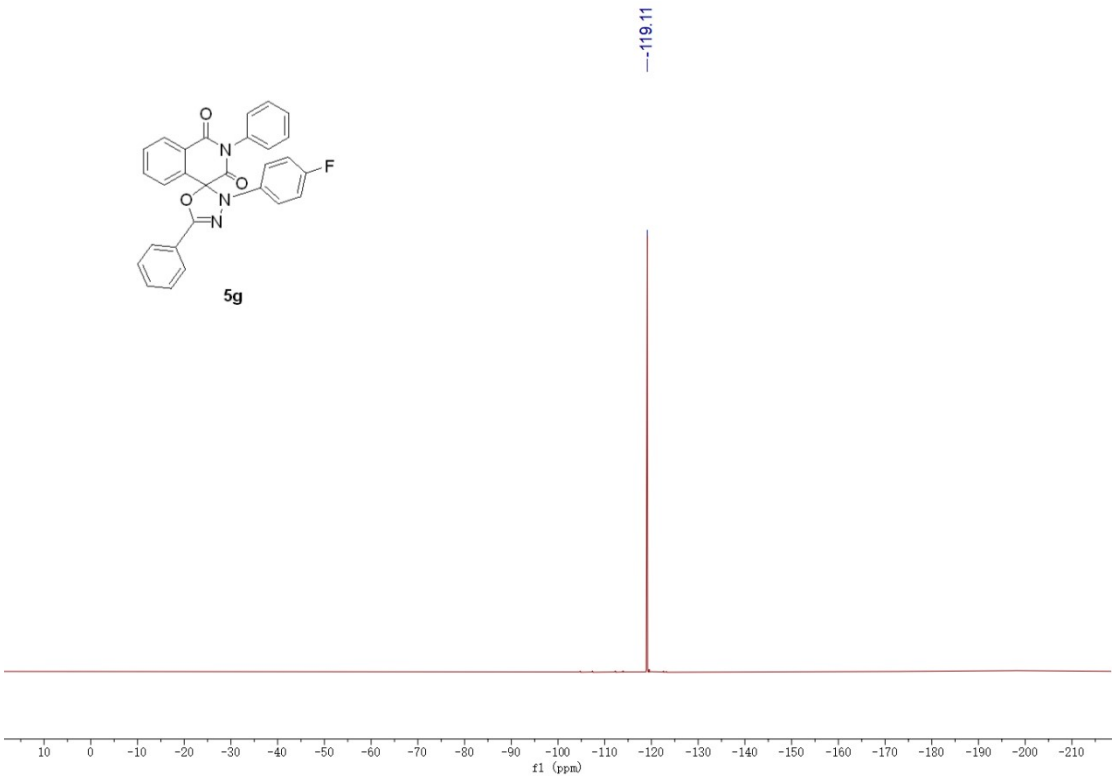
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



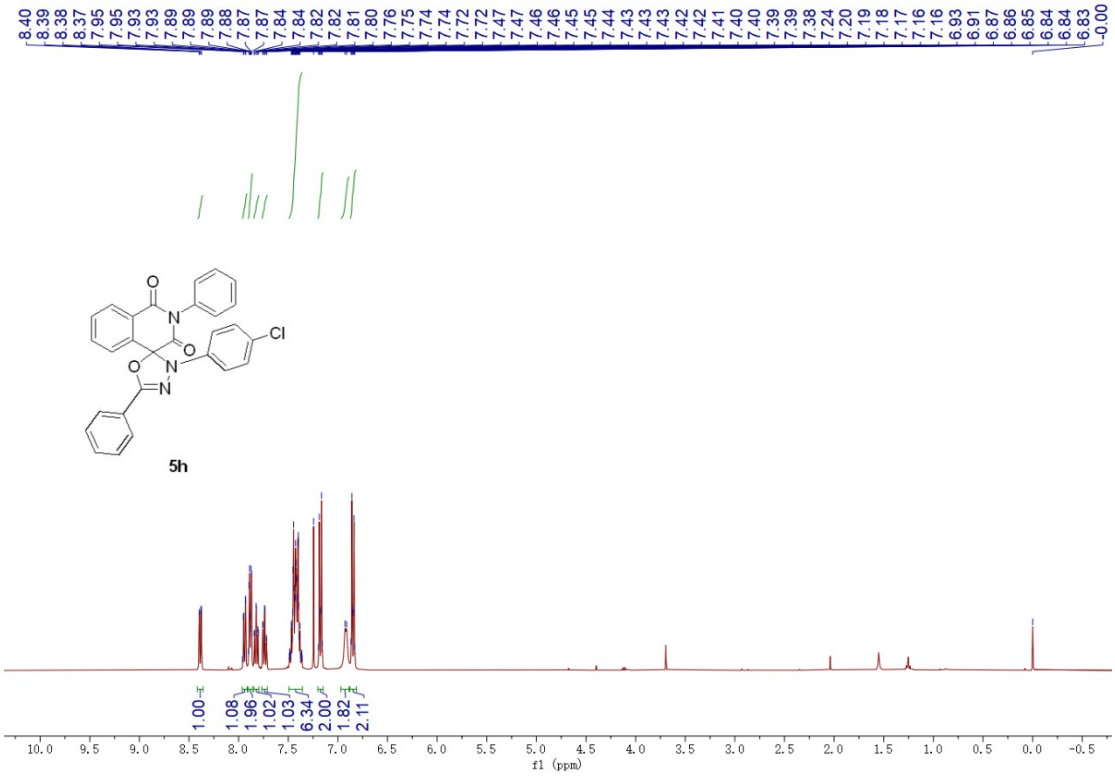
^{19}F NMR ($CDCl_3$, 376 MHz)



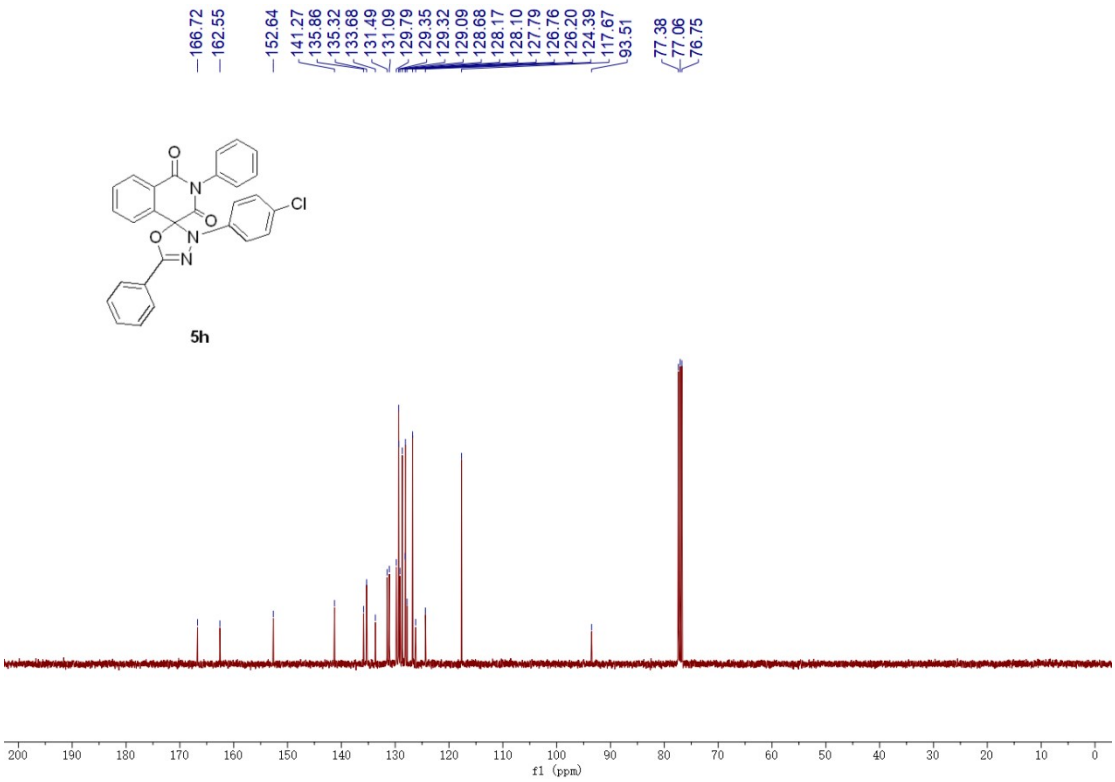
3'-(4-chlorophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5h)

^{1}H NMR ($CDCl_3$, 400 MHz)



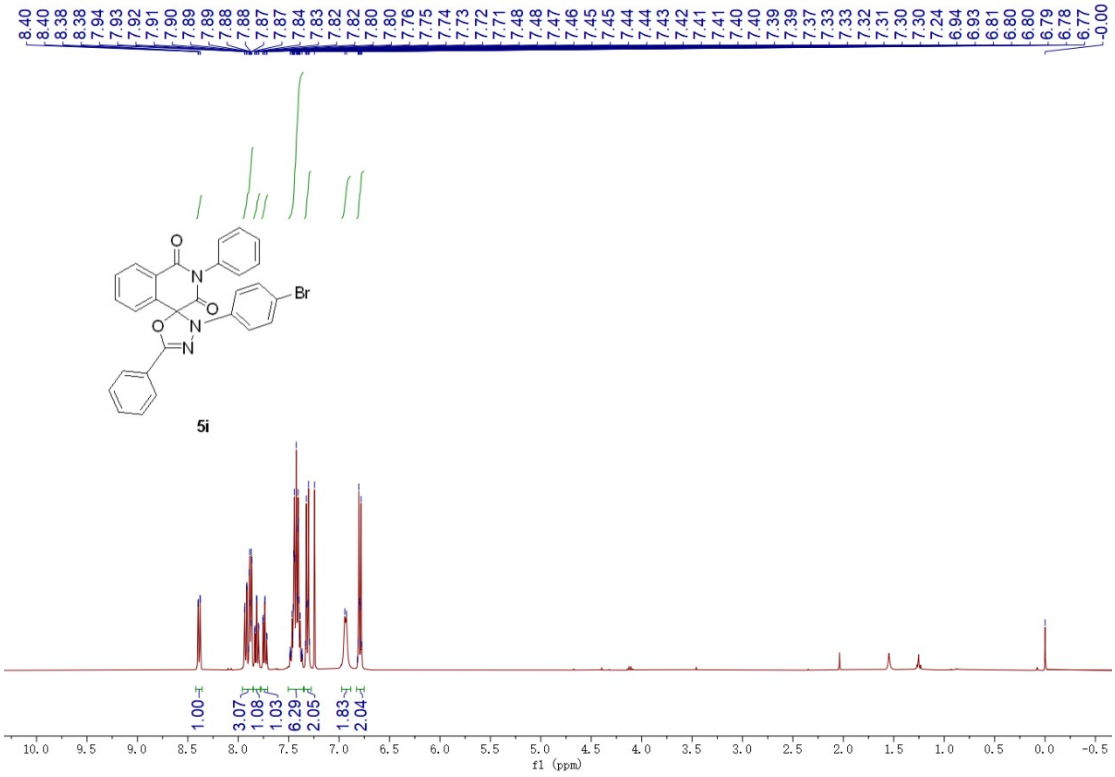
^{13}C NMR ($CDCl_3$, 100 MHz)



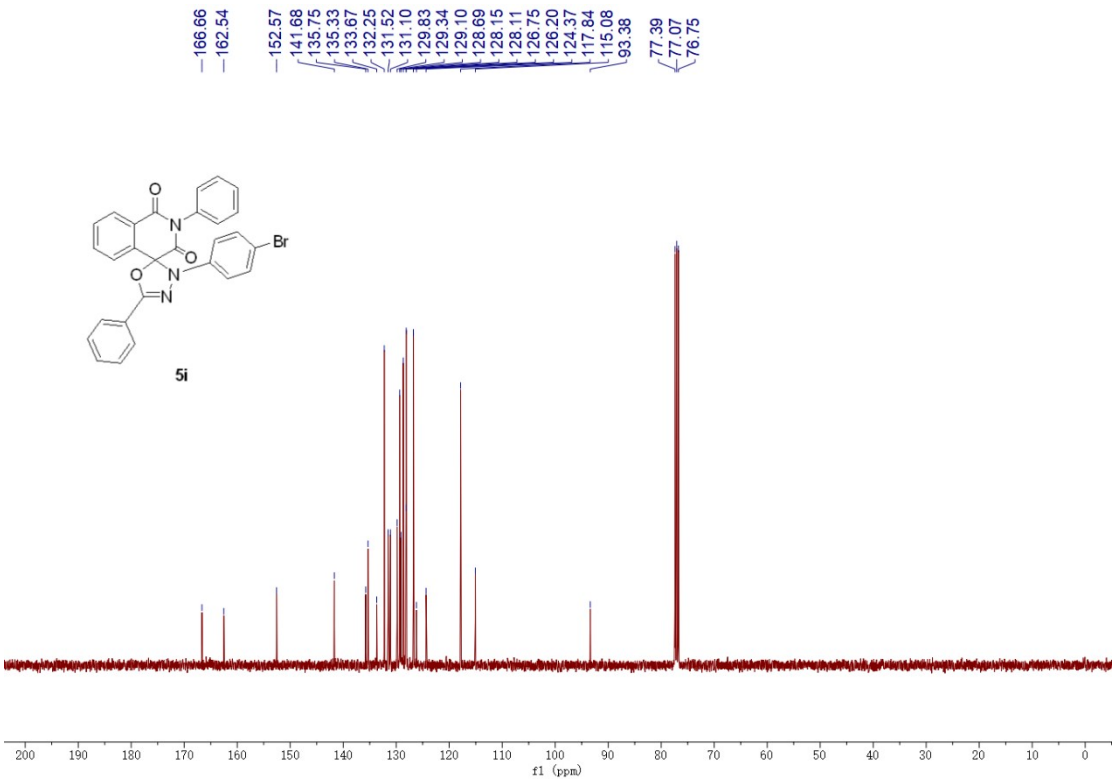
3'-(4-bromophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5i)

^{1}H NMR ($CDCl_3$, 400 MHz)



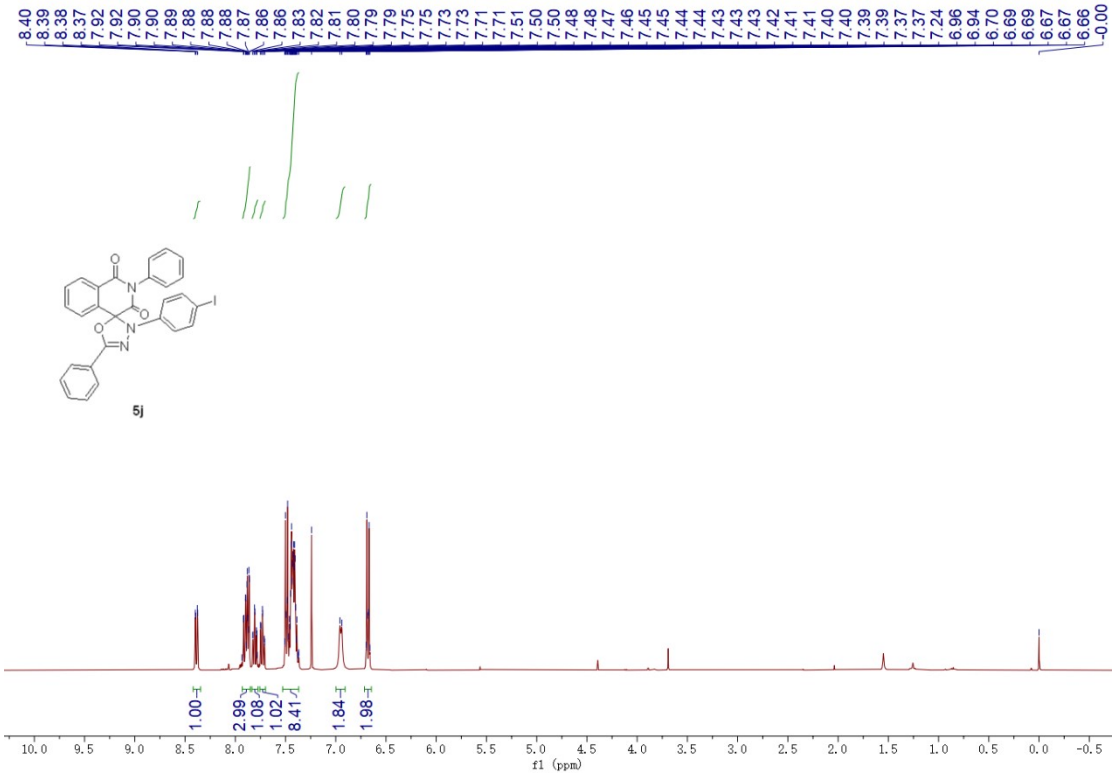
^{13}C NMR ($CDCl_3$, 100 MHz)



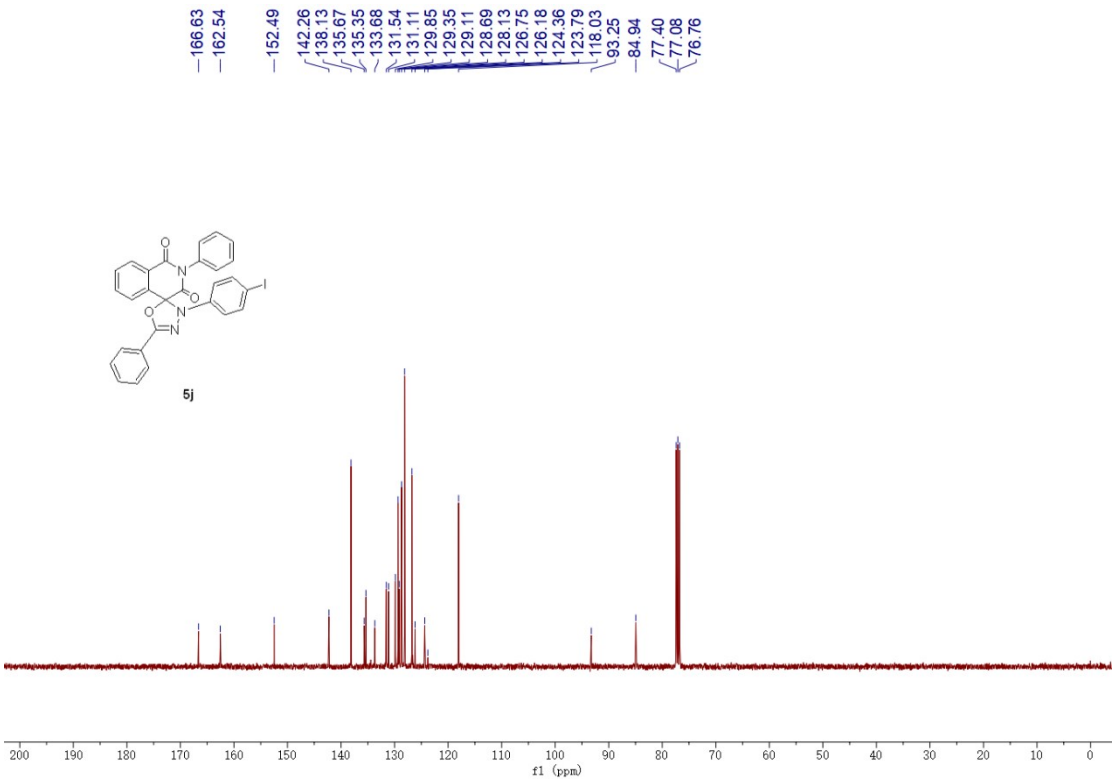
3'-(4-iodophenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5j)

^{1}H NMR ($CDCl_3$, 400 MHz)



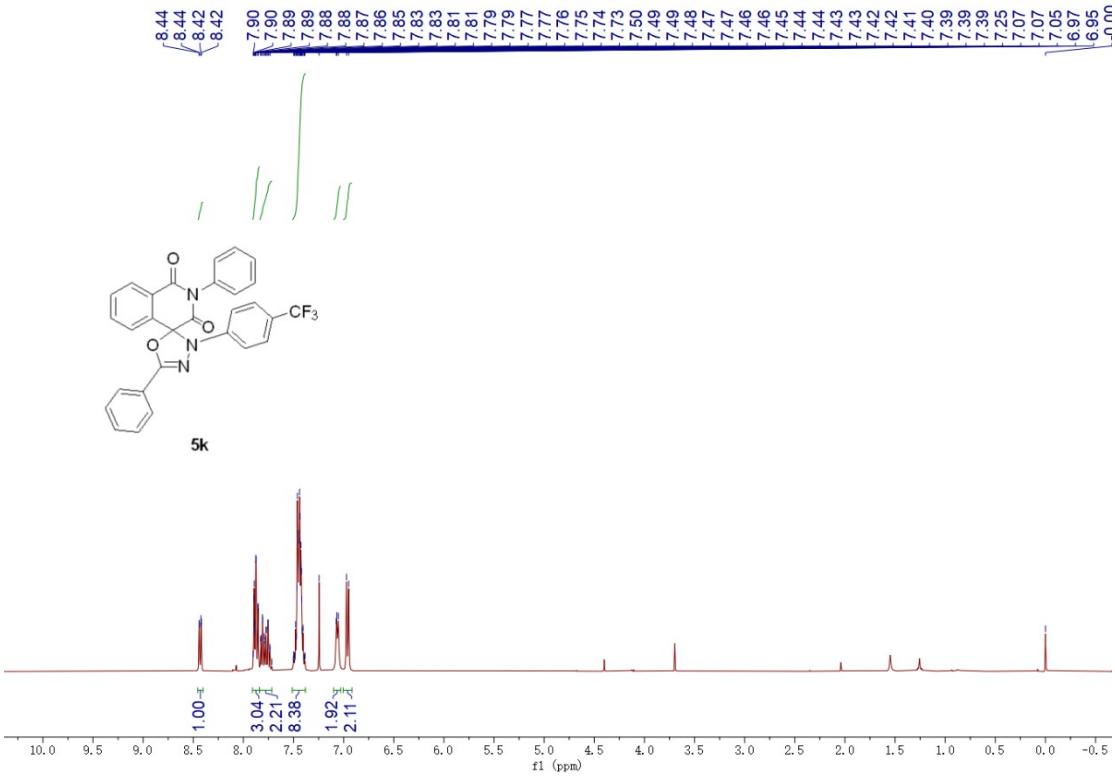
^{13}C NMR ($CDCl_3$, 100 MHz)



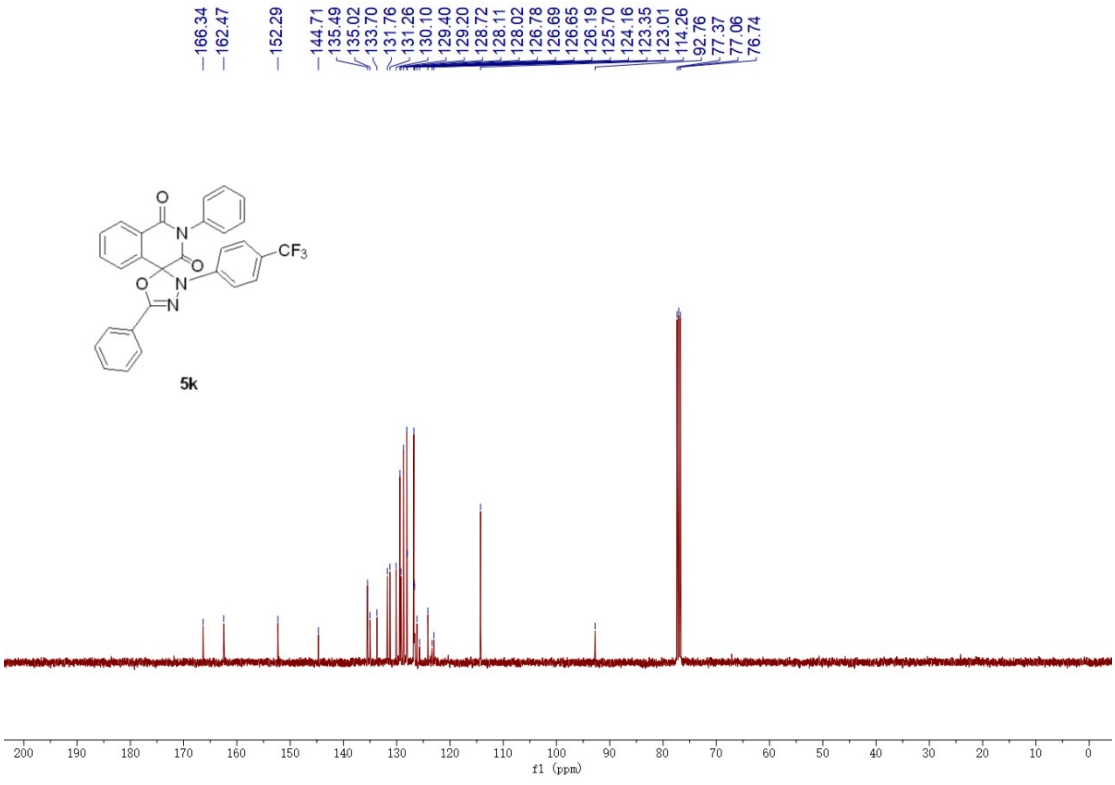
2,5'-diphenyl-3'-(4-(trifluoromethyl)phenyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5k)

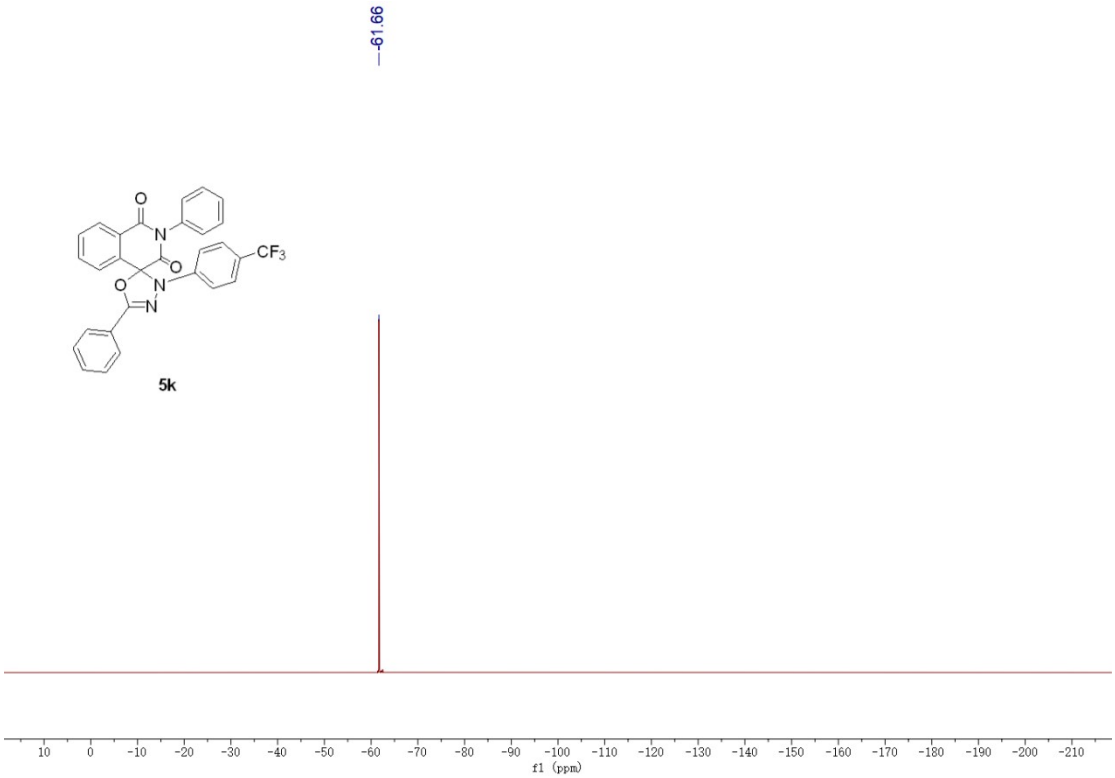
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



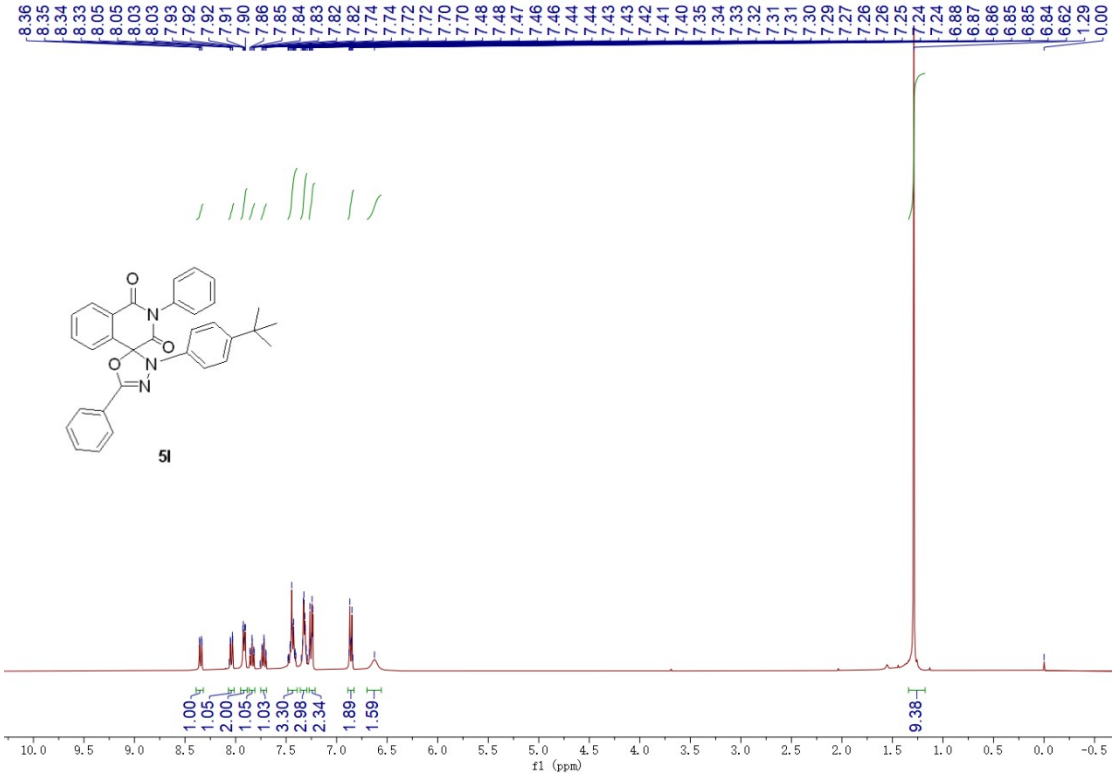
^{19}F NMR ($CDCl_3$, 376 MHz)



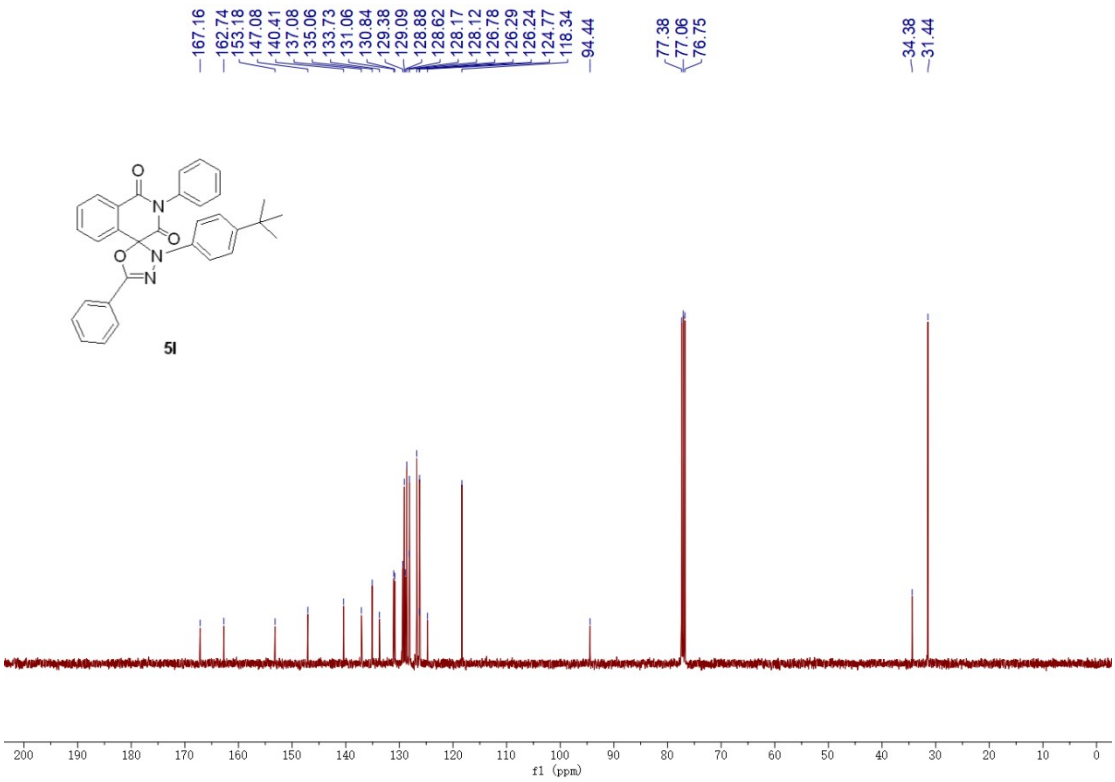
3'-(4-(tert-butyl)phenyl)-2,5'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5l)

^{1}H NMR ($CDCl_3$, 400 MHz)



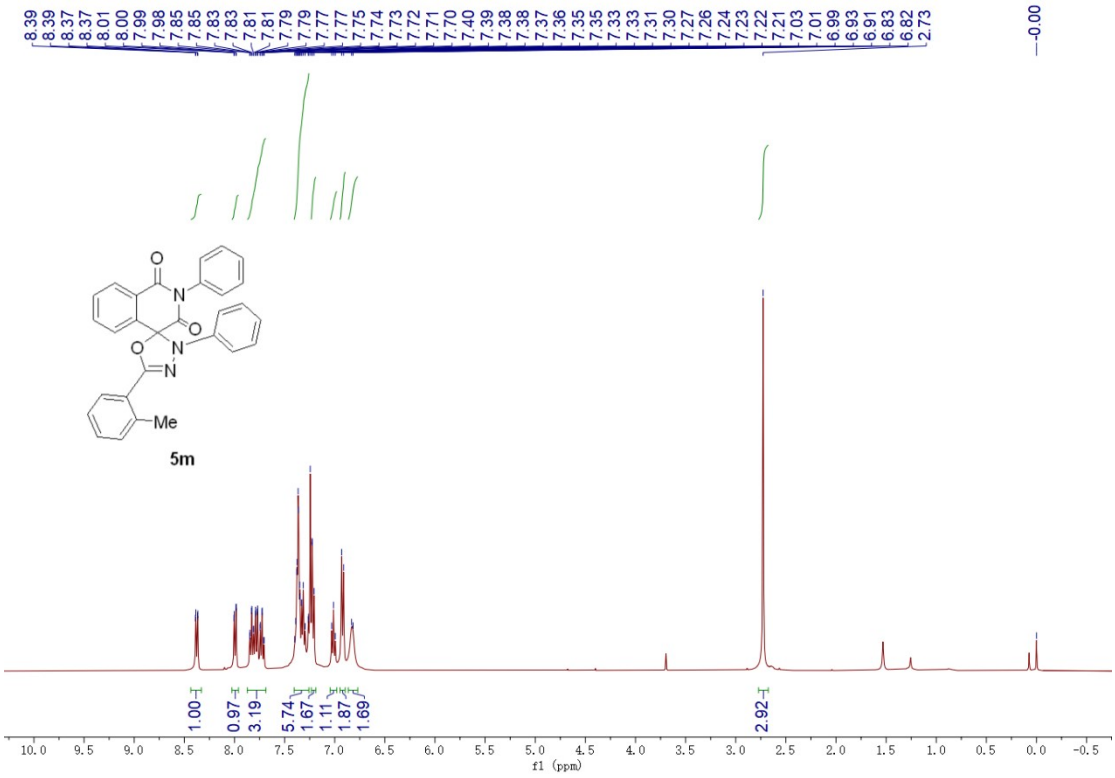
^{13}C NMR ($CDCl_3$, 100 MHz)



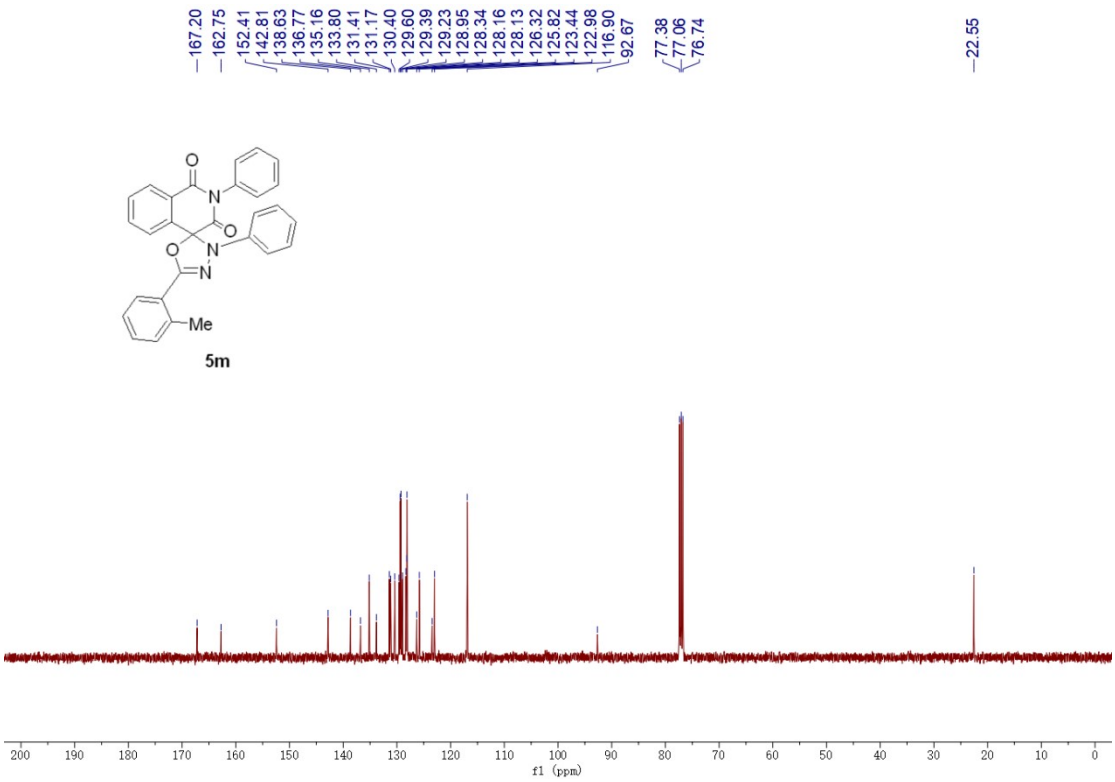
2,3'-diphenyl-5'-(o-tolyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-

1,3(2*H*)-dione (5m)

^{1}H NMR ($CDCl_3$, 400 MHz)



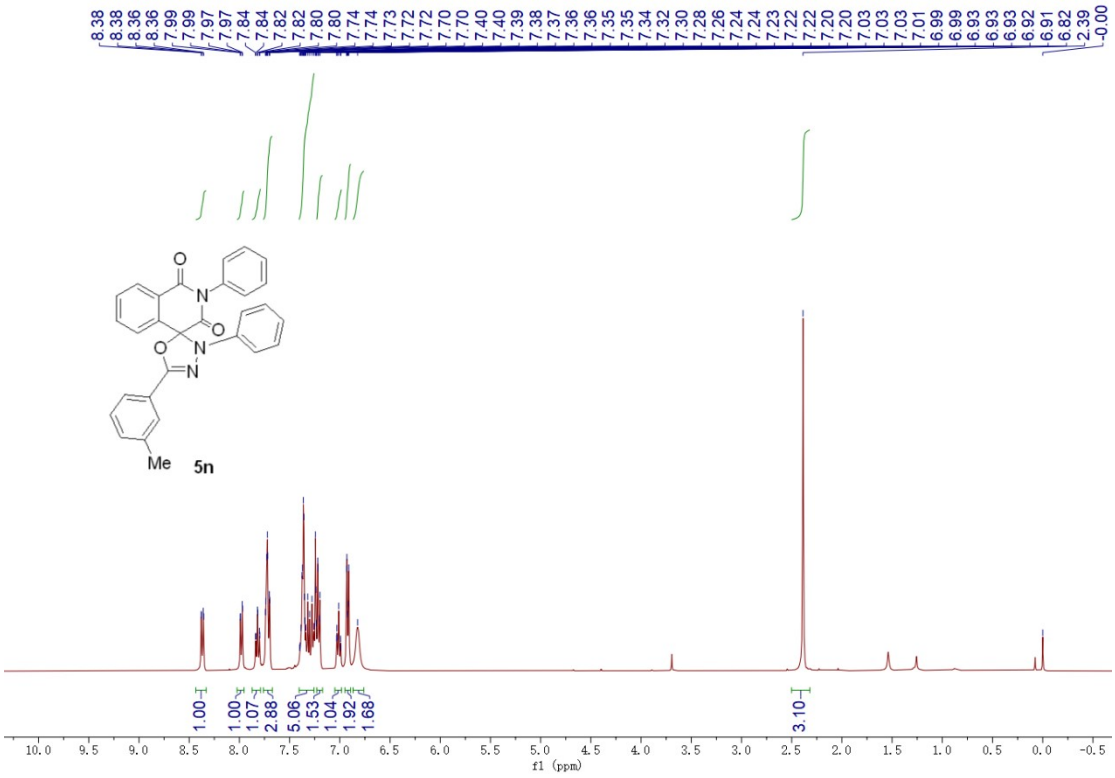
^{13}C NMR ($CDCl_3$, 100 MHz)



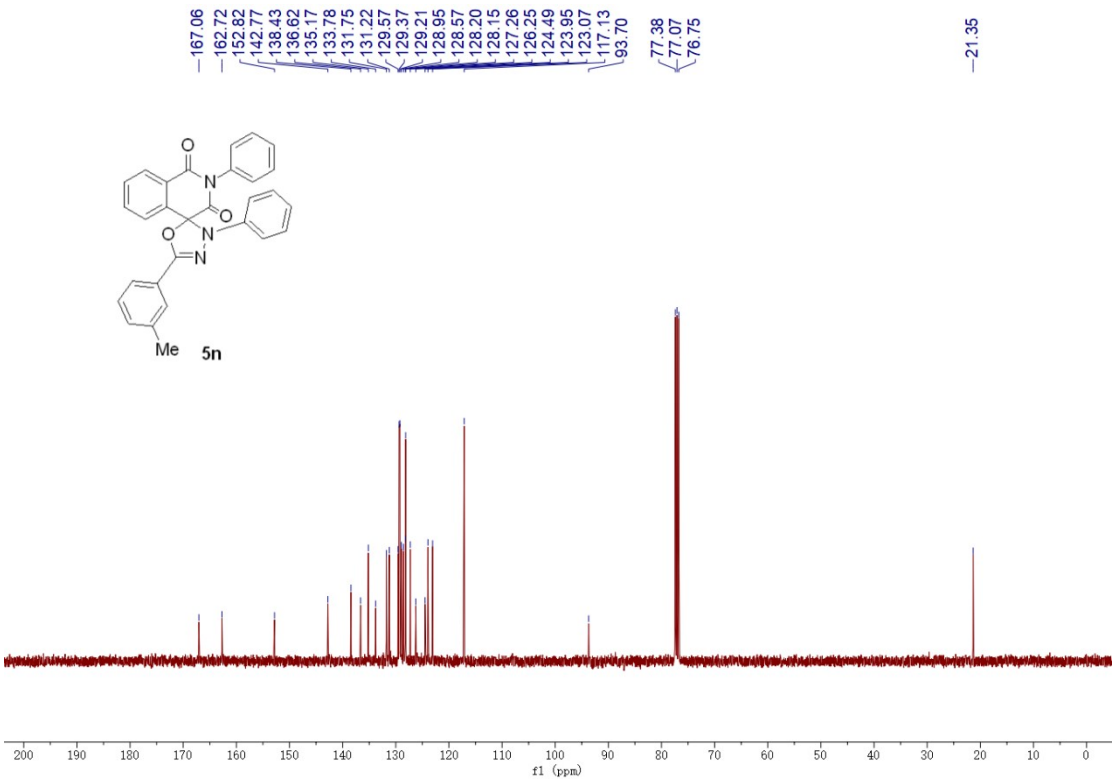
2,3'-diphenyl-5'-(m-tolyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-

1,3(2*H*)-dione (5n)

^{1}H NMR ($CDCl_3$, 400 MHz)



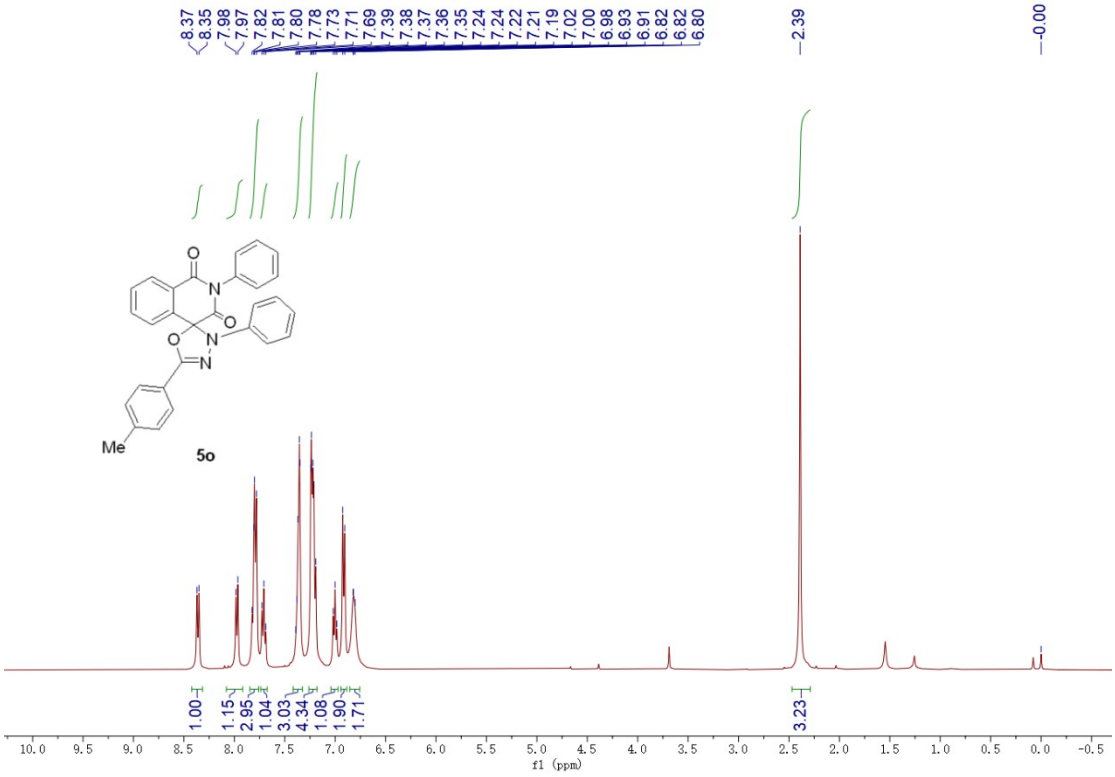
^{13}C NMR ($CDCl_3$, 100 MHz)



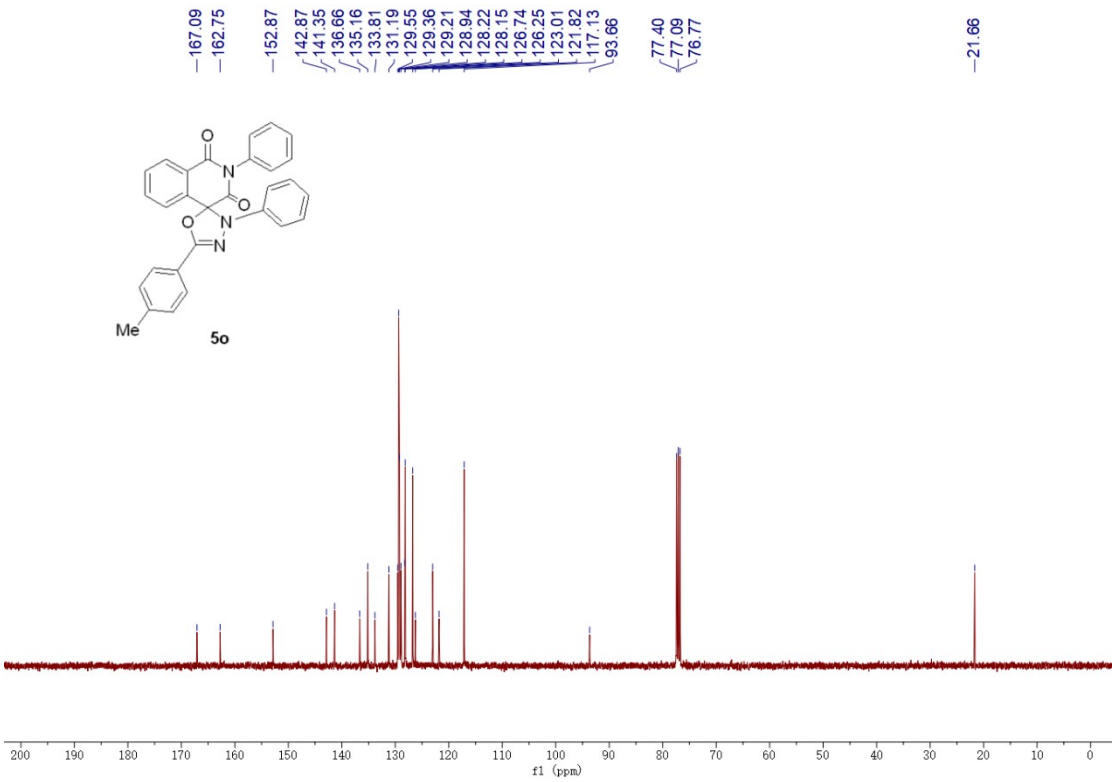
2,3'-diphenyl-5'-(p-tolyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-

1,3(2*H*)-dione (5o)

^{1}H NMR ($CDCl_3$, 400 MHz)



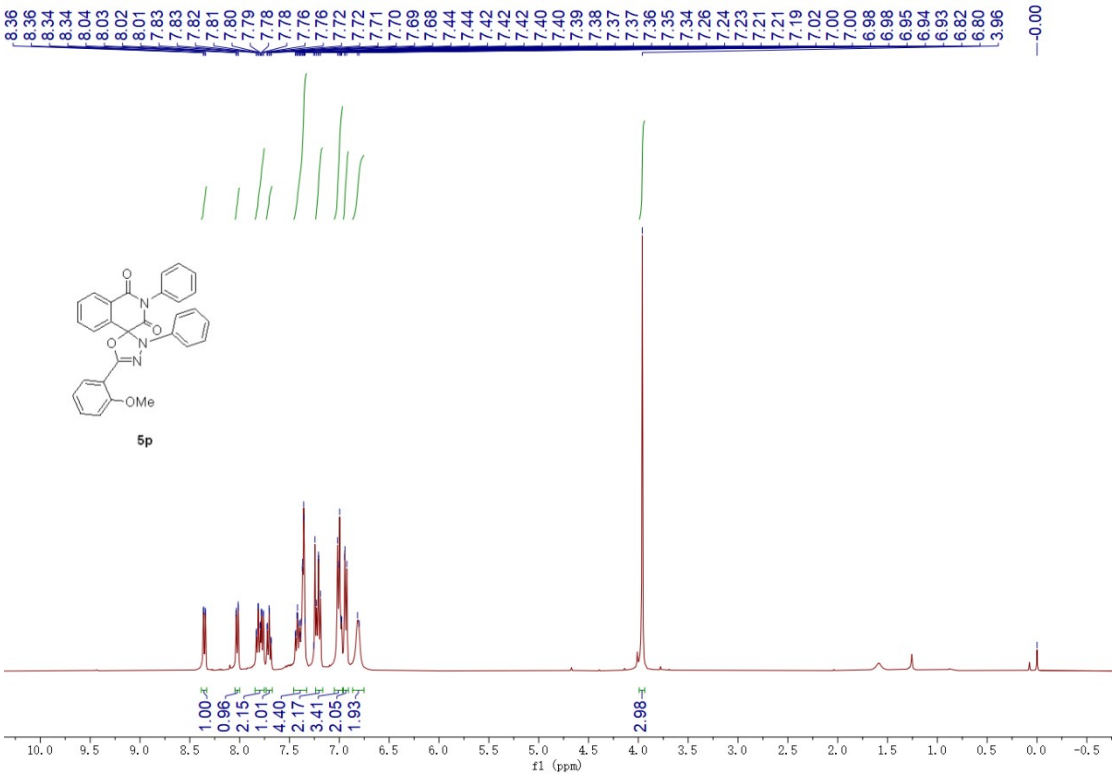
^{13}C NMR ($CDCl_3$, 100 MHz)



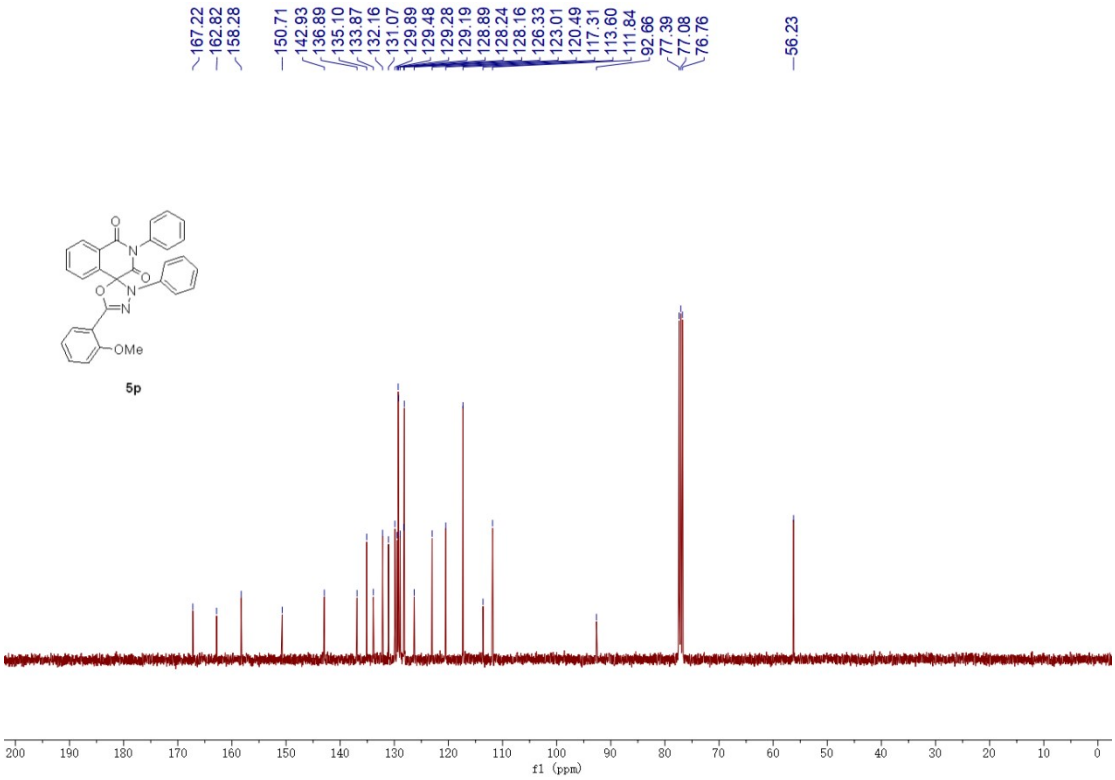
5'-(2-methoxyphenyl)-2,3'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5p)

^{1}H NMR ($CDCl_3$, 400 MHz)



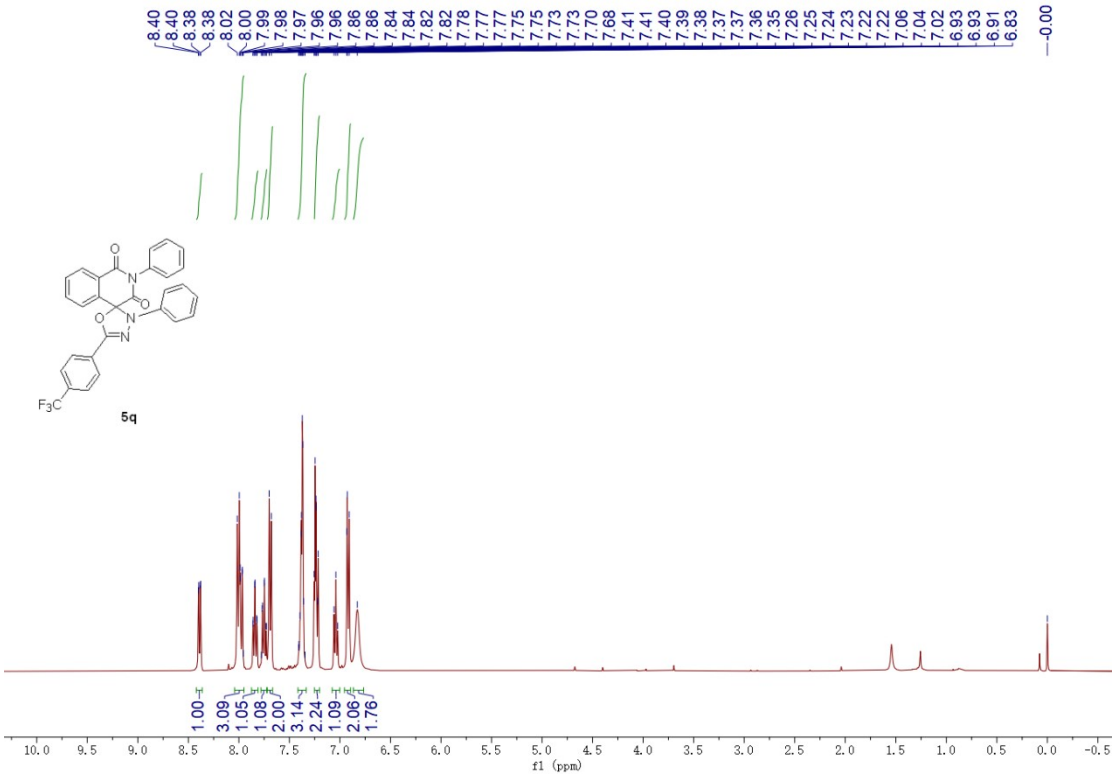
^{13}C NMR ($CDCl_3$, 100 MHz)



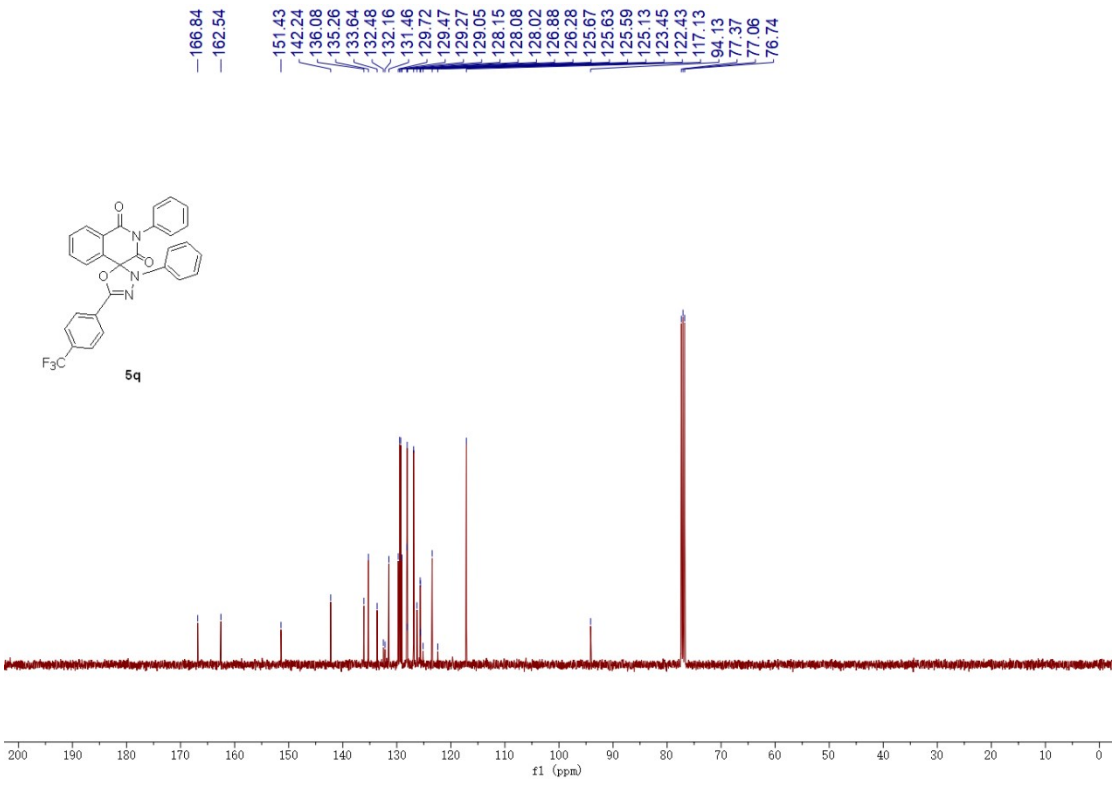
2,3'-diphenyl-5'-(4-(trifluoromethyl)phenyl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5q)

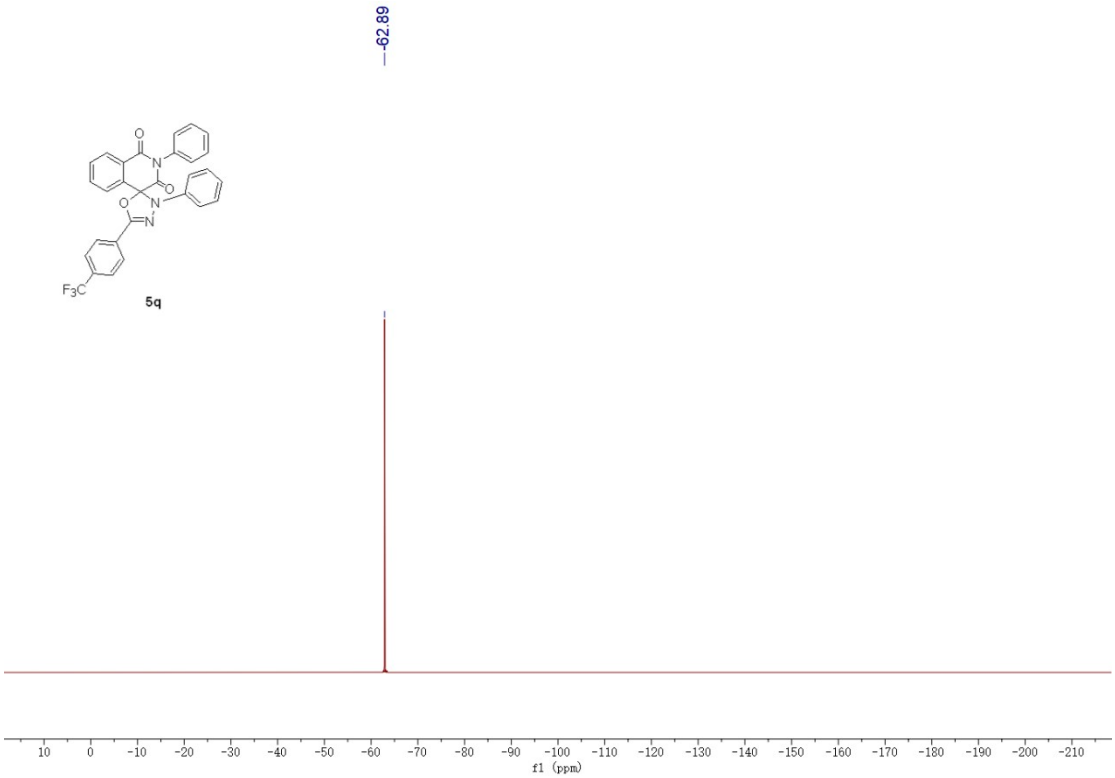
^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)



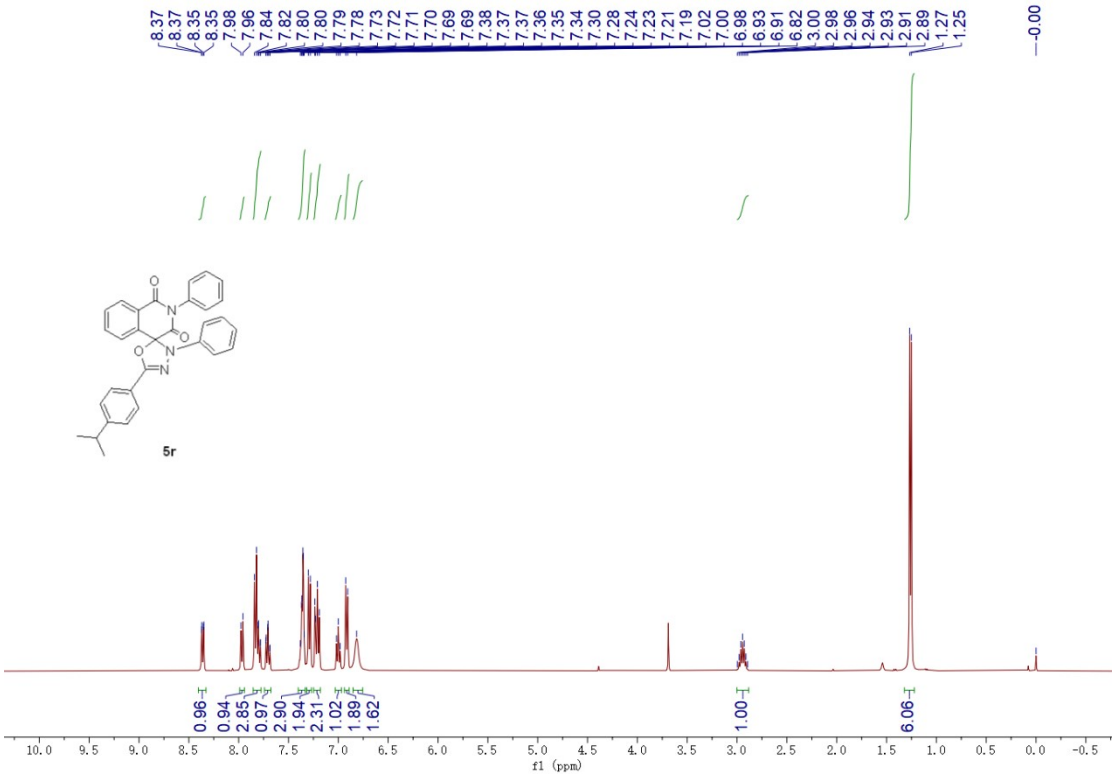
^{19}F NMR ($CDCl_3$, 376 MHz)



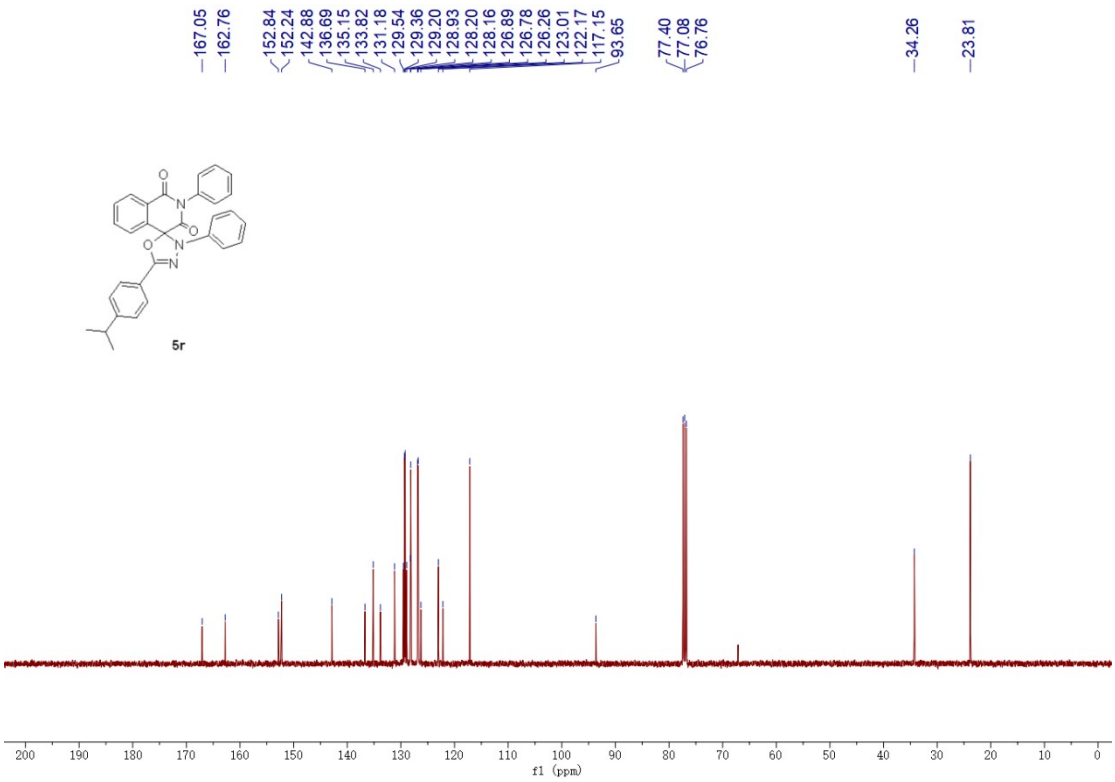
5'-(4-isopropylphenyl)-2,3'-diphenyl-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5r)

^{1}H NMR ($CDCl_3$, 400 MHz)



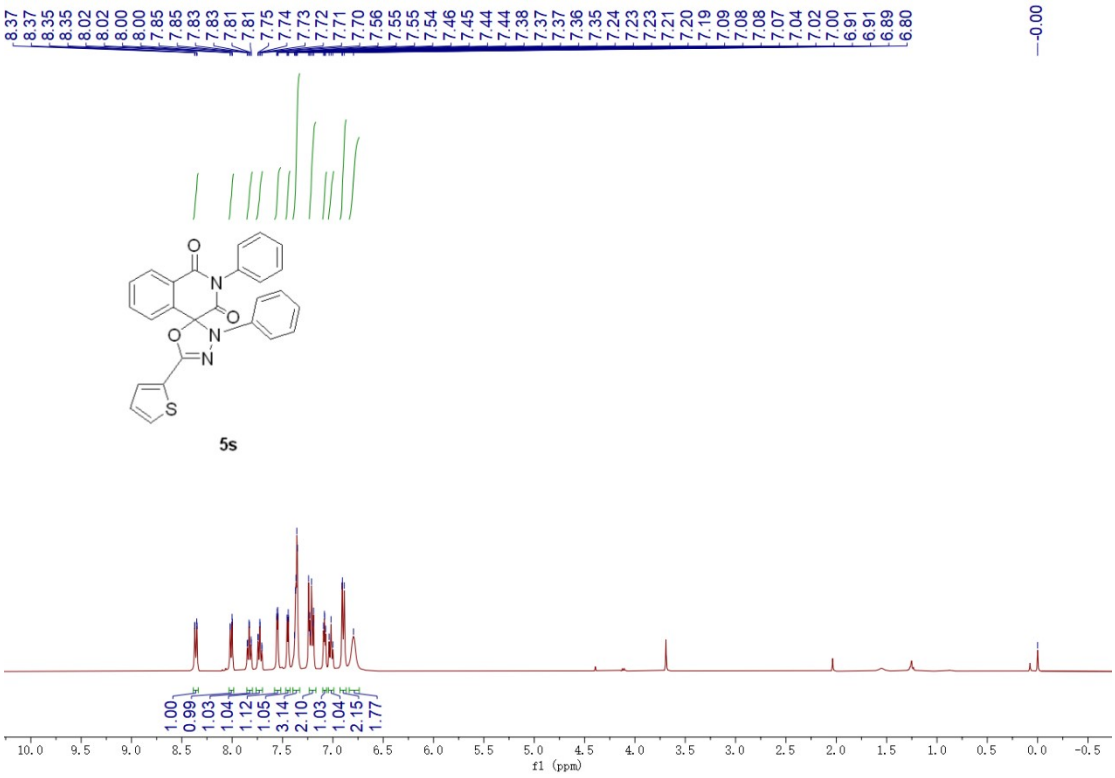
^{13}C NMR ($CDCl_3$, 100 MHz)



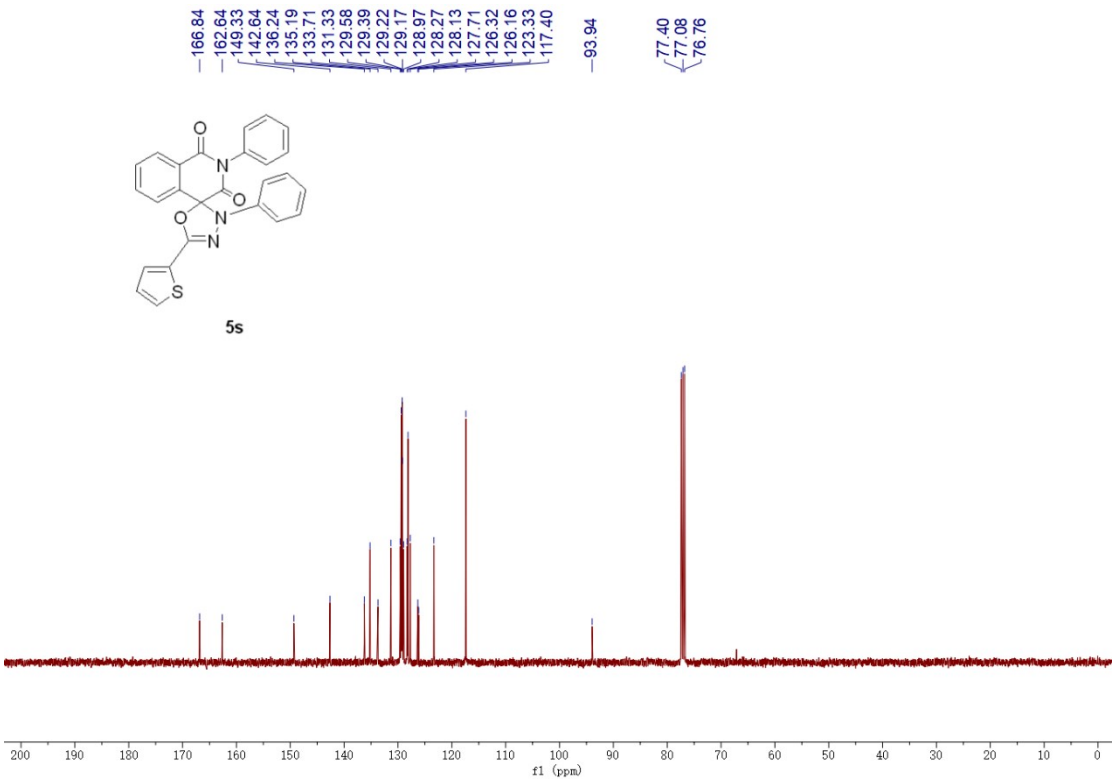
2,3'-diphenyl-5'-(thiophen-2-yl)-1*H*,3'*H*-spiro[isoquinoline-4,2'-

[1,3,4]oxadiazole]-1,3(2*H*)-dione (5s)

^{1}H NMR ($CDCl_3$, 400 MHz)



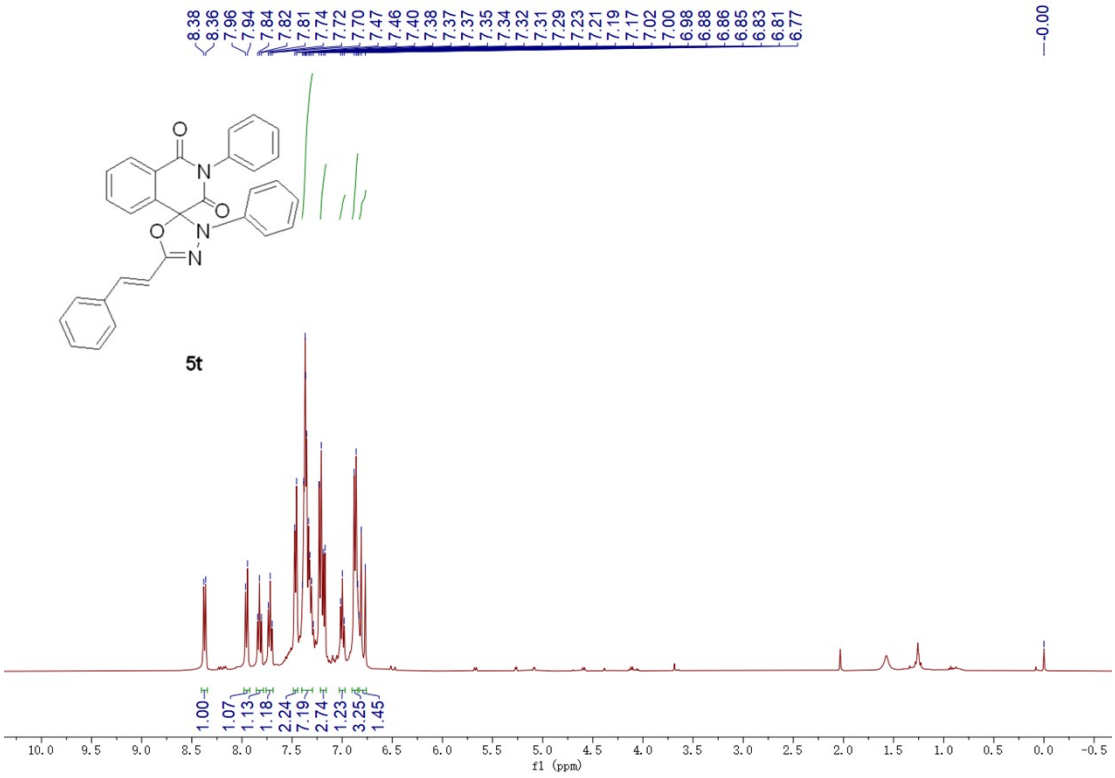
^{13}C NMR ($CDCl_3$, 100 MHz)



2,3'-diphenyl-5'-styryl-1H,3'H-spiro[isoquinoline-4,2'-[1,3,4]oxadiazole]-1,3(2H)-

dione (5t)

^{1}H NMR ($CDCl_3$, 400 MHz)



^{13}C NMR ($CDCl_3$, 100 MHz)