Supplementary Information

for

Diastereoselective Radical Cascade Cyclization to Access Indole-Fused Diazepine Derivatives

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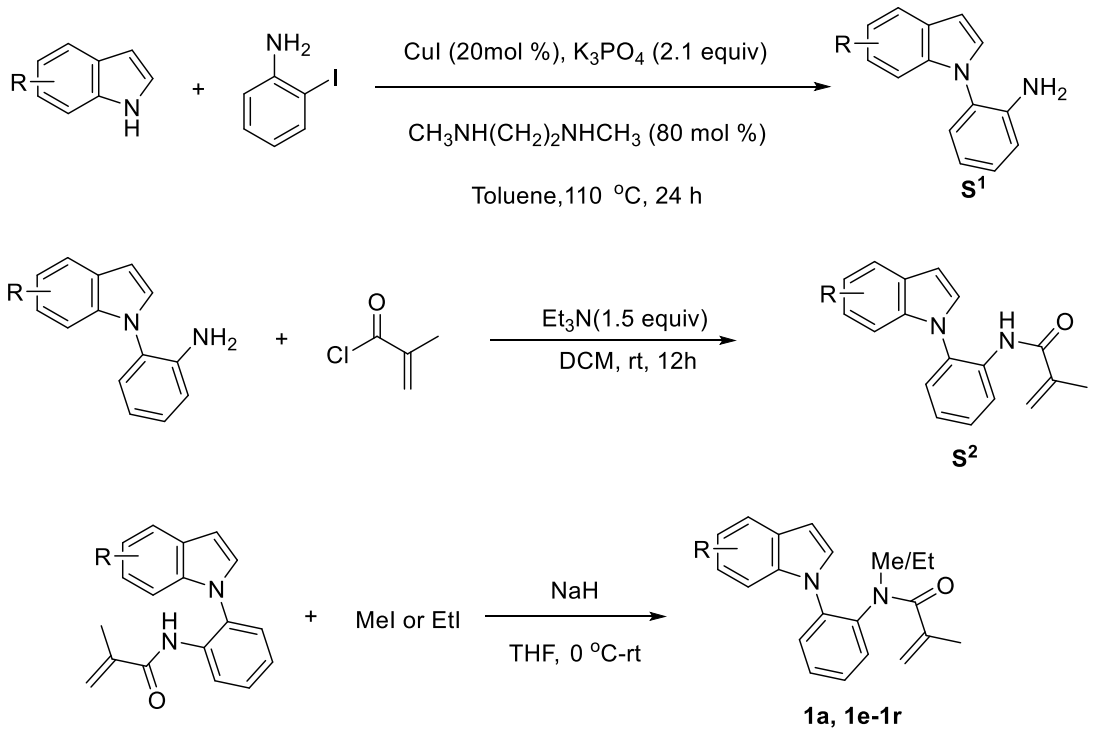
1 General information

Unless otherwise noted, materials obtained from commercial suppliers were used without further purification. Flash column chromatography was performed over silica gel (200-300 mesh). The ^{13}C NMR spectra signal of Materials *o*-indolo acrylamides **1** is very weak, so it is not involved. ^{1}H NMR, ^{13}C NMR, ^{31}P NMR and ^{19}F NMR spectra were recorded at ambient temperature using Bruker 400M spectrometers and JEOL 500M spectrometers, chemical shifts (in ppm) were referenced to $CDCl_3$ (δ = 7.26 ppm) as internal standards.^{13}C NMR spectra were obtained by using the same NMR spectrometers and were calibrated with $CDCl_3$ (δ = 77.0 ppm). Data for ^{1}H NMR are recorded as following abbreviations: multiplicity (s = singlet, d = doublet, t = triplet, q = quarter, m = multiplet), coupling constant (*J*, Hz). High resolution mass spectroscopy (HRMS) analyses were performed at an Exactive Plus (Thermo Scientific) or Agilent Mass Spectrometer. The X-ray crystal structure was measured on the Agilent Gemini E diffractometer instrument.

2 Procedures for the preparation of starting materials

2.1 General procedure A: Synthesis of 1a, 1e-1r:

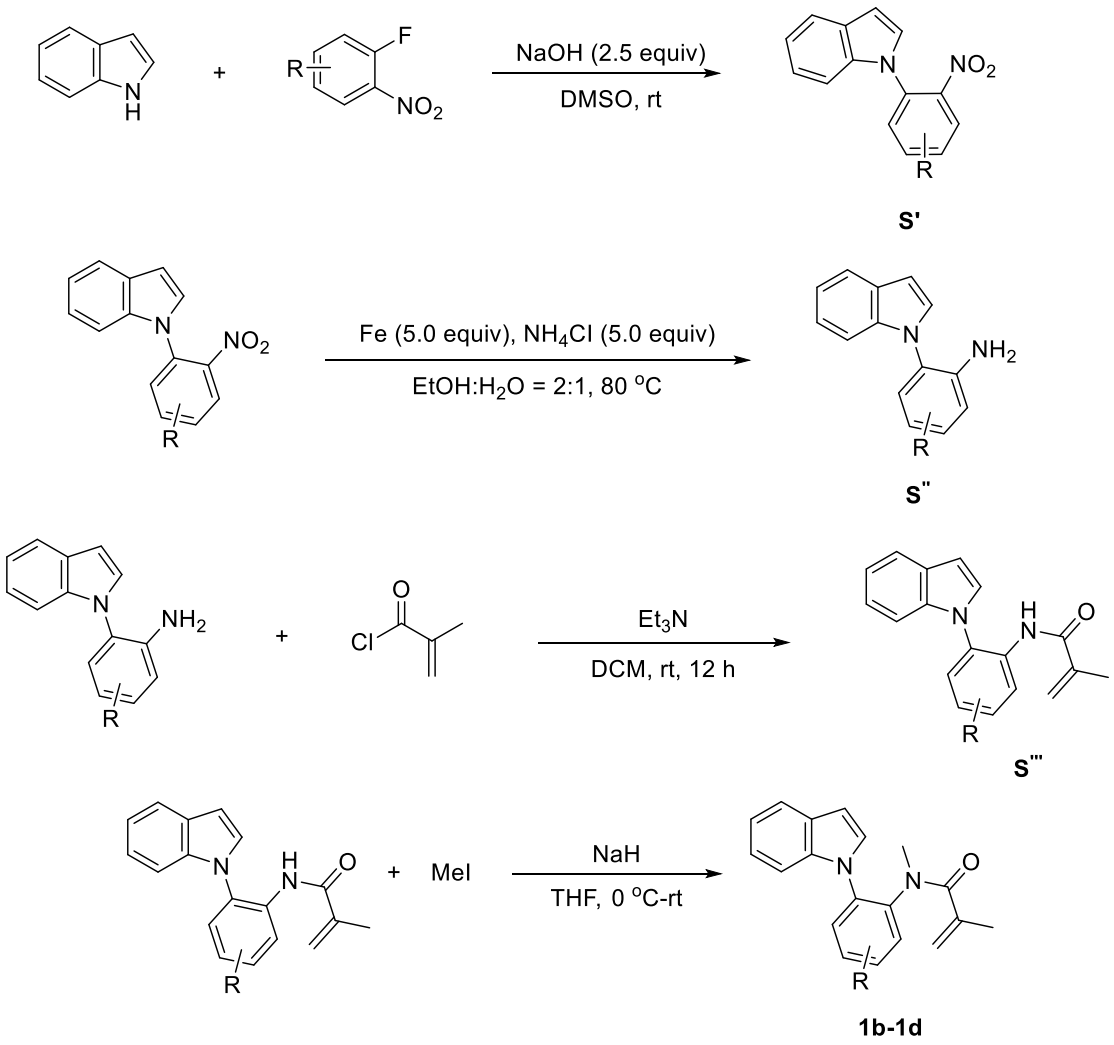


A Schlenk bottle was charged with indole (5.0 mmol, 1.0 equiv), 2-Iodoaniline (1.5 equiv), CuI (20 mol%), K_3PO_4 (2.1 equiv). The bottle was evacuated and filled with argon for three cycles. Then, toluene (10.0 mL) and N,N'-dimethylethylenediamine (80 mol%) were added under argon. The reaction was allowed to stir at 110°C (oil bath) for 24 hours. After completion (TLC), the reaction mixture was cooled to room temperature and then diluted with ethyl acetate and filtered through a plug of silica gel. The filtrate was concentrated and the resulting residue was purified by column chromatography, eluting with PE/EA (v/v = 10:1) to afford the desired product **S[1]**.

To a solution of **S[1]** (1.0 equiv) in anhydrous DCM at room temperature was added Et_3N (1.5 equiv) and methacryloyl chloride (1.5 equiv). After being stirred at room temperature under air for 12 h, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with DCM. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with PE/EA (v/v = 10:1) to afford the desired product **S[2]**.

To a solution of **S[2]** (1.0 equiv) in anhydrous THF at 0 °C was slowly added NaH (5.0 equiv), and then MeI or EtI (1.5 equiv) was added dropwisely. The mixture was then stirred at room temperature under air for 4 h. After the reaction was completed (monitored by TLC), followed by quenched with water and the aqueous phase was extracted with DCM. The combined organic layers were then dried over Na_2SO_4, and concentrated under reduced pressure, and the residue was purified by silica gel chromatography to obtain the corresponding product**.**

2.1 General procedure B: Synthesis of 1b-1d:



A mixture of indole (10mmol), substituted aryl fluoride (10 mmol) and NaOH (25 mmol) in DMSO (20 mL) was stirred for 2 h. Upon completion of reaction mixture was poured in H_2O and extracted with ethyl acetate. The aqueous layer was extracted with ethyl acetate and the combined organic

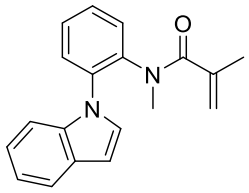
layers were dried over Na_2SO_4 and concentrated in vacuo to corresponding **S'**. The crude was directly used for the next step.

A mixture of **S'**, ammonium chloride and Iron powder in alcohol/H_2O (v/v = 2:1) was stirred at 80 °C for 1h. Upon completion of reaction, the reaction mixture was filtered through a bed of celite and extracted with H_2O and EA. The combined organic layers were washed with Na_2SO_4 and concentred under vacuum to **S''**. The crude was directly used for the next step.

To a solution of **S''** (1.0 equiv) in anhydrous DCM at room temperature was added Et_3N (1.5 equiv) and methacryloyl chloride (1.5 equiv). After being stirred at room temperature under air for 12 h, the reaction was quenched with saturated NH_4Cl aqueous solution and extracted with DCM. The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with PE/EA (v/v = 10:1) to afford the desired product **S'''**.

To a solution of **S'''** (1.0 equiv) in anhydrous THF at 0 °C was slowly added NaH (5.0 equiv), and then MeI or EtI (1.5 equiv) was added dropwisely. The mixture was then stirred at room temperature under air for 4 h. After the reaction was completed (monitored by TLC), followed by quenched with water and the aqueous phase was extracted with DCM. The combined organic layers were then dried over Na_2SO_4, and concentrated under reduced pressure, and the residue was purified by silica gel chromatography to obtain the corresponding product**.**

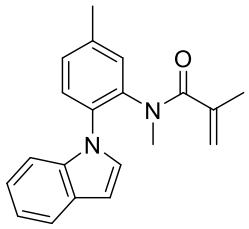
***N*-(2-(1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1a)**



White solid, mp: 120-121 ºC. Yield: 68%.

^{1}H NMR (500 MHz, DMSO-*D*$_6$) δ 7.71–7.61 (m, 2H), 7.50 (s, 3H), 7.25 (s, 1H), 7.20–7.05 (m, 3H), 6.68 (d, *J* = 3.3 Hz, 1H), 4.85 (s, 1H), 4.52 (s, 1H), 3.22 (s, 2H), 2.73 (s, 1H), 1.67 (s, 1H), 0.72 (s, 2H). **HRMS (ESI)** calcd for $C_{19}H_{19}N_2O^+$ $[M+H]^+$: 291.1492, found: 291.1486.

***N*-(2-(1*H*-indol-1-yl)-5-methylphenyl)-*N*-methylmethacrylamide (1b)**

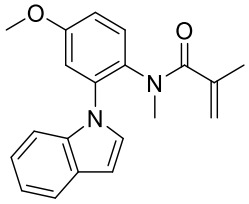


White solid, mp: 106-107 ºC. Yield: 46 %.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 6.8 Hz, 1H), 7.39 (d, *J* = 7.0 Hz, 1H), 7.29–7.20 (m, 3H), 7.20–7.11 (m, 2H), 7.05 (s, 1H), 6.66 (s, 1H), 4.91 (s, 1H), 4.73 (s, 1H), 3.20 (s, 2H), 2.69 (s, 1H), 2.45 (s, 3H), 1.83 (s, 1H), 1.02 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ $[M+H]^+$: 305.1648, found: 305.1643.

***N*-(2-(1*H*-indol-1-yl)-4-methoxyphenyl)-*N*-methylmethacrylamide (1c)**

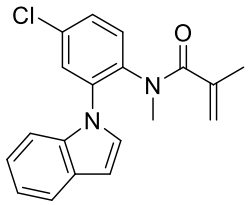


White solid, mp: 86-87 ºC. Yield: 46 %.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.66 (d, *J* = 7.7 Hz, 1H), 7.38–7.28 (m, 2H), 7.23–7.14 (m, 2H), 7.10–7.02 (m, 2H), 6.95 (d, *J* = 7.6 Hz, 1H), 6.68 (s, 1H), 4.90 (s, 1H), 4.68 (s, 1H), 3.84 (s, 3H), 3.19 (s, 2H), 2.68 (s, 1H), 1.85 (s, 1H), 1.06 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O_2^+$ $[M+H]^+$: 321.1598, found: 321.1592.

***N*-(4-chloro-2-(1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1d)**

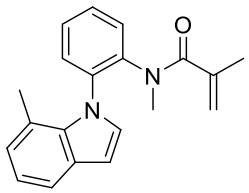


White solid, mp: 88-89 ºC. Yield: 36 %

^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 8.0 Hz, 1H), 7.53 (d, *J* = 2.3 Hz, 1H), 7.38 (s, 2H), 7.30–7.20 (m, 2H), 7.20–7.13 (m, 1H), 7.05 (s, 1H), 6.69 (d, *J* = 3.3 Hz, 1H), 4.96 (s, 1H), 4.72 (s, 1H), 3.20 (s, 2H), 2.68 (s, 1H), 1.83 (s, 1H), 1.02 (s, 2H).

HRMS (ESI) calcd for $C_{19}H_{18}ClN_2O^+$ $[M+H]^+$: 325.1102, found: 325.1098.

***N*-methyl-*N*-(2-(7-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1e)**

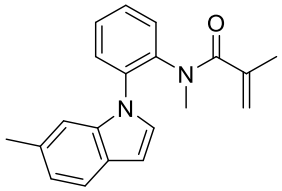


White solid, mp: 101-102 ºC. Yield: 86%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.52 (d, *J* = 7.9 Hz, 1H), 7.50–7.28 (m, 4H), 7.11–7.03 (m, 2H), 6.94 (d, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 3.2 Hz, 1H), 5.08 (s, 1H), 4.79 (s, 1H), 2.85 (s, 3H), 2.04 (s, 3H), 1.93–1.49 (m, 3H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ $[M+H]^+$: 305.1648, found: 305.1644.

***N*-methyl-*N*-(2-(6-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1f)**

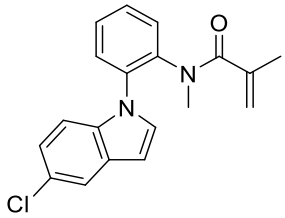


White solid, mp: 121-122 ºC. Yield: 64%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.67–7.49 (m, 2H), 7.42 (s, 3H), 7.17–6.86 (m, 3H), 6.62 (d, *J* = 3.3 Hz, 1H), 4.94 (s, 1H), 4.75 (s, 1H), 3.16 (s, 2H), 2.69 (s, 1H), 2.42 (s, 3H), 1.85 (s, 1H), 1.12 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ $[M+H]^+$: 305.1648, found: 305.1644.

***N*-(2-(5-chloro-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1g)**

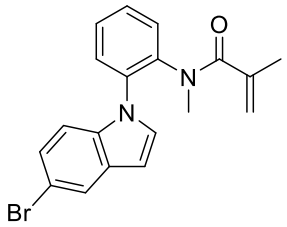


White solid, mp: 130-131 ºC. Yield: 66%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.61 (s, 1H), 7.45 (s, 4H), 7.13 (s, 3H), 6.61 (d, *J* = 3.3 Hz, 1H), 4.90 (s, 1H), 4.67 (s, 1H), 3.41–2.57 (m, 3H), 1.82 (s, 1H), 1.03 (s, 2H).

HRMS (ESI) calcd for $C_{19}H_{18}ClN_2O^+$ $[M+H]^+$: 325.1102, found: 325.1097.

***N*-(2-(5-bromo-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1h)**

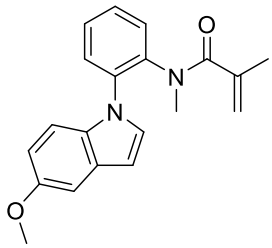


White solid, mp: 116-117 ºC. Yield: 68%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.78 (d, *J* = 1.9 Hz, 1H), 7.50–7.39 (m, 4H), 7.30 – 6.99 (m, 3H), 6.61 (d, *J* = 3.3 Hz, 1H), 4.91 (s, 1H), 4.69 (s, 1H), 3.44–2.61 (m, 3H), 1.82 (s, 1H), 1.05 (s, 2H).

HRMS (ESI) calcd for $C_{19}H_{18}BrN_2O^+$ $[M+H]^+$: 369.0597, found: 369.0593.

***N*-(2-(5-methoxy-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1i)**

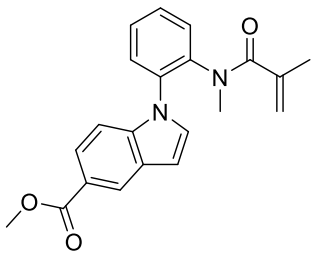


White solid, mp: 119-120 ºC. Yield: 85%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.50 (d, *J* = 4.5 Hz, 1H), 7.47–7.38 (m, 4H), 7.18–6.99 (m, 3H), 6.61 (d, *J* = 3.1 Hz, 1H), 4.93 (s, 1H), 4.73 (s, 1H), 3.20 (s, 2H), 2.71 (s, 1H), 2.47 (s, 3H), 1.96–1.79 (m, 1H), 1.10 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O_2^+$ $[M+H]^+$: 321.1598, found: 321.1589.

methyl 1-(2-(*N*-methylmethacrylamido)phenyl)-1*H*-indole-5-carboxylate (1j)

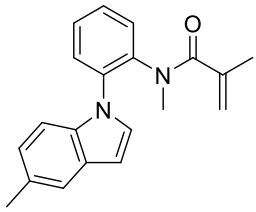


White solid, mp: 114-115 ºC. Yield: 63%

^{1}H NMR (500 MHz, Chloroform-d) δ 8.42 (s, 1H), 7.89 (d, *J* = 7.0 Hz, 1H), 7.54–7.41 (m, 4H), 7.22 (d, *J* = 8.7 Hz, 1H), 7.13 (s, 1H), 6.76 (s, 1H), 4.89 (s, 1H), 4.67 (s, 1H), 3.93 (s, 3H), 3.24 (s, 2H), 2.76 (s, 1H), 1.79 (s, 1H), 0.96 (s, 2H).

HRMS (ESI) calcd for $C_{21}H_{21}N_2O_3^+$ $[M+H]^+$: 349.1547, found: 349.1541.

***N*-methyl-*N*-(2-(5-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1k)**

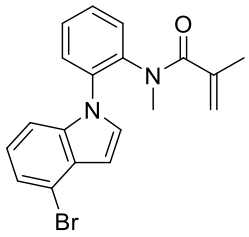


White solid, mp: 120-121 ºC. Yield: 77%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.57–7.47 (m, 1H), 7.44 (s, 2H), 7.41 (s, 2H), 7.14 (d, *J* = 8.4 Hz, 1H), 7.08–6.98 (m, 2H), 6.59 (d, *J* = 3.3 Hz, 1H), 4.92 (s, 1H), 4.72 (s, 1H), 3.18 (s, 2H), 2.70 (s, 1H), 2.45 (s, 3H), 1.86 (s, 1H), 1.09 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ $[M+H]^+$: 305.1648, found: 305.1643.

***N*-(2-(4-bromo-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1l)**

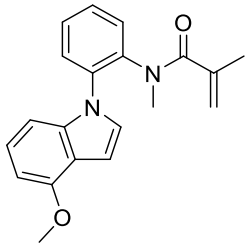


White solid, mp: 105-106 ºC. Yield: 86%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.58–7.49 (m, 1H), 7.42 (s, 3H), 7.13–7.05 (m, 3H), 7.00–6.91 (m, 1H), 6.70 (d, *J* = 3.5 Hz, 1H), 4.93 (s, 1H), 4.73 (s, 1H), 3.19 (s, 2H), 2.71 (s, 1H), 1.87 (s, 1H), 1.32–0.92 (m, 2H).

HRMS (ESI) calcd for $C_{19}H_{18}BrN_2O^+$ $[M+H]^+$: 369.0597, found: 369.0601.

***N*-(2-(4-methoxy-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1m)**

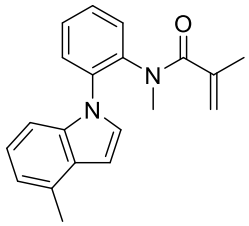


White solid, mp: 128-129 ºC. Yield: 76%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.53–7.36 (m, 4H), 7.13–6.97 (m, 2H), 6.89–6.82 (m, 1H), 6.78 (d, *J* = 3.3 Hz, 1H), 6.57 (d, *J* = 7.8 Hz, 1H), 4.94 (s, 1H), 4.74 (s, 1H), 3.98 (s, 3H), 3.16 (s, 2H), 2.69 (s, 1H), 1.86 (s, 1H), 1.14 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O_2^+$ $[M+H]^+$: 321.1598, found: 321.1592.

***N*-methyl-*N*-(2-(4-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1n)**

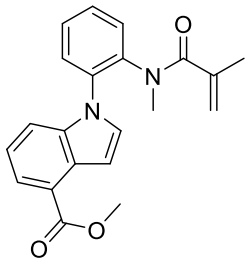


White solid, mp: 132-133 ºC. Yield: 57%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.52 (d, *J* = 7.9 Hz, 1H), 7.49–7.37 (m, 4H), 7.12–7.03 (m, 2H), 6.94 (d, *J* = 7.2 Hz, 1H), 6.63 (d, *J* = 3.3 Hz, 1H), 5.08 (s, 1H), 4.79 (s, 1H), 2.85 (s, 3H), 2.04 (s, 3H), 1.93–1.49 (m, 3H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ $[M+H]^+$: 305.1648, found: 305.1645.

methyl 1-(2-(*N*-methylmethacrylamido)phenyl)-1*H*-indole-4-carboxylate (1o)

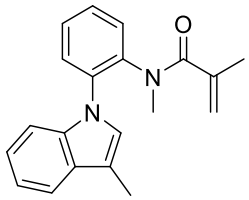


White solid, mp: 108-109 ºC. Yield: 76%

^{1}H NMR (500 MHz, DMSO-*D*6) δ 8.33 (d, J = 1.6 Hz, 1H), 7.83 – 7.69 (m, 2H), 7.60 – 7.49 (m, 3H), 7.39 (s, 1H), 7.22 (d, J = 8.8 Hz, 1H), 6.85 (d, J = 3.3 Hz, 1H), 4.85 (s, 1H), 4.49 (s, 1H), 3.85 (s, 3H), 3.26 (s, 2H), 2.85 (s, 1H), 1.61 (s, 1H), 0.66 (s, 2H).

HRMS (ESI) calcd for $C_{21}H_{21}N_2O_3^+$ $[M+H]^+$: 349.1547, found: 349.1541.

***N*-methyl-*N*-(2-(3-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1p)**

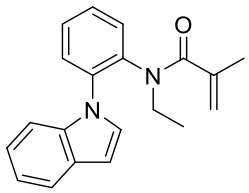


White solid, mp: 86-87 ºC. Yield: 57%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.61 (d, *J* = 6.8 Hz, 1H), 7.53–7.34 (m, 4H), 7.25–7.21 (m, 1H), 7.20–7.15 (m, 2H), 6.87 (s, 1H), 4.93 (s, 1H), 4.73 (s, 1H), 3.20 (s, 2H), 2.68 (s, 1H), 2.37 (s, 3H), 1.88 (s, 1H), 1.11 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ $[M+H]^+$: 305.1648, found: 305.1645.

***N*-(2-(1*H*-indol-1-yl)phenyl)-*N*-ethylmethacrylamide (1q)**

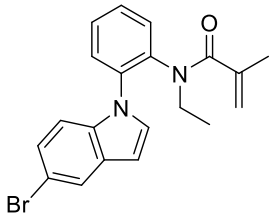


White solid, mp: 103-104 °C. Yield: 67%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.75–7.63 (m, 1H), 7.59–7.32 (m, 4H), 7.25 (s, 1H), 7.22–7.10 (m, 3H), 6.66 (s, 1H), 5.19–4.70 (m, 2H), 4.35–2.37 (m, 2H), 1.92 (s, 1H), 1.18 (s, 3H), 0.80 (s, 2H).

HRMS (ESI) calcd for $C_{20}H_{21}N_2O^+$ [M+H]$^+$: 305.1648, found: 305.1645.

***N*-(2-(5-bromo-1*H*-indol-1-yl)phenyl)-*N*-ethylmethacrylamide (1r)**

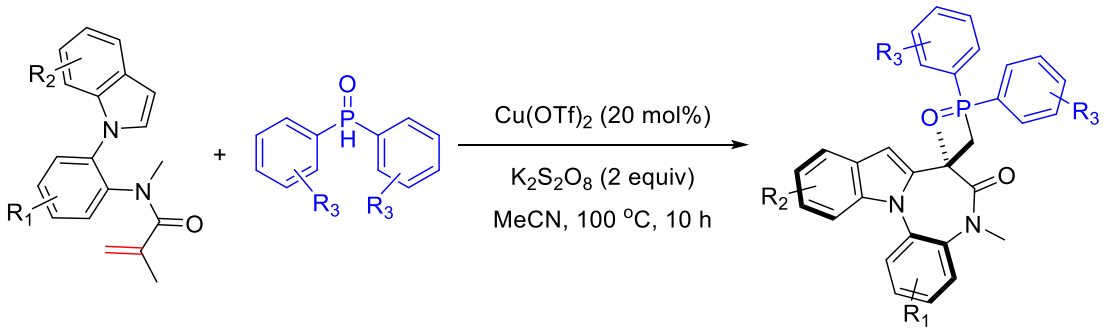


White solid, mp: 102-103 °C. Yield: 58%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 (d, *J* = 1.9 Hz, 1H), 7.61–7.34 (m, 4H), 7.26–7.22 (m, 2H), 7.10 (d, *J* = 8.7 Hz, 1H), 6.59 (s, 1H), 5.27–4.64 (m, 2H), 4.24–2.48 (m, 2H), 1.90 (s, 1H), 1.35–0.62 (m, 5H).

HRMS (ESI) calcd for $C_{20}H_{20}BrN_2O^+$ [M+H]$^+$: 383.0754, found: 383.0749.

3 General procedure for Cu-catalyzed phosphorylation cyclization reaction

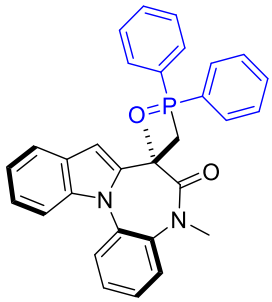


1 **2** **3**

In the glove box filled with high-purity argon, a 10 mL Young tube was charged with N-Methyl-aryl acrylamide (0.2 mmol, 1 equiv.), diphenylphosphine oxide (0.4 mmol, 2 equiv.), $Cu(OTf)_2$ (9.8 mg, 20 mol%), $K_2S_2O_8$ (108.1 mg, 2 equiv), and 4 mL MeCN. Then, the tube was removed from

the glove box. The reaction mixture was stirred at 100 ℃ in an oil bath for 10 h. Upon completion, proper amount of silica gel was added to the reaction mixture. After removal of the solvent, the crude reaction mixture was purified on silica gel (ethyl acetate) to afford the desired products.

7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3a)



White solid, mp: 287-288 ºC. Yield: 86%.

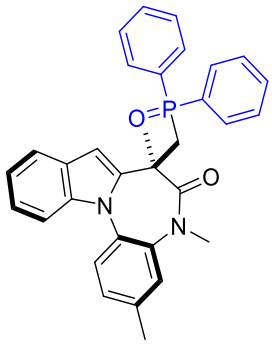
^{1}H NMR (500 MHz, Chloroform-d) δ 7.59 (d, *J* = 7.0 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 1H), 7.49 (d, *J* = 7.3 Hz, 1H), 7.47–7.41 (m, 1H), 7.41–7.27 (m, 10H), 7.24–7.10 (m, 4H), 6.50 (s, 1H), 3.29 (s, 3H), 2.55 (dd, *J* = 15.6, 13.5 Hz, 1H), 2.33 (dd, *J* = 15.5, 9.7 Hz, 1H), 1.97 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.47.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.8 (d, *J* = 7.7 Hz), 143.1 (d, *J* = 9.3 Hz), 137.3, 135.8, 132.4, 131.6 (dd, *J* = 25.3, 2.7 Hz), 130.9 (d, *J* = 9.5 Hz), 130.6 (d, *J* = 9.1 Hz), 129.0, 128.3 (dd, *J* = 19.2, 11.6 Hz), 126.8, 125.7, 124.4, 124.0, 122.5, 121.1 (d, *J* = 13.8 Hz), 110.6, 101.8, 44.9 (d, *J* = 3.4 Hz), 38.5, 34.7 (d, *J* = 66.8 Hz), 24.1.

HRMS (ESI) calcd for $C_{31}H_{28}N_2O_2P^+[M+H]^+$: 491.1883; Found: 491.1874.

7-((diphenylphosphoryl)methyl)-3,5,7-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3b)



White solid, mp: 142-143 ºC. Yield: 84%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.57 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 8.8 Hz, 1H), 7.46–7.39 (m, 4H), 7.39–7.31 (m, 4H), 7.31–7.27 (m, 1H), 7.24 (d, *J* = 2.9 Hz, 1H), 7.24–7.20 (m, 1H), 7.20–7.15 (m, 2H), 7.15–7.10 (m, 2H), 6.46 (s, 1H), 3.29 (s, 3H), 2.57 (dd, *J* = 15.6, 13.7 Hz, 1H), 2.44 (s, 3H), 2.32 (dd, *J* = 15.6, 9.5 Hz, 1H), 1.92 (s, 3H).

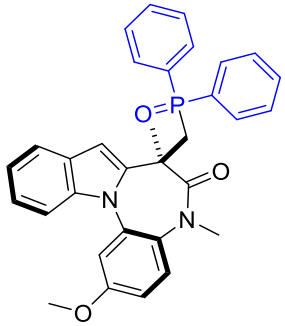
^{1}H NMR (500 MHz, $CDCl_3$) δ 2.57 (dd, *J* = 15.6, 13.7 Hz, 1H), 2.32 (dd, *J* = 15.6, 9.5 Hz, 1H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.51.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.7 (d, *J* = 6.9 Hz), 143.1 (d, *J* = 9.7 Hz), 137.1 (d, *J* = 10.5 Hz), 135.8, 134.2, 133.4, 132.9, 131.6 (dd, *J* = 12.3, 2.6 Hz), 130.9 (d, *J* = 9.4 Hz), 130.5 (d, *J* = 9.2 Hz), 129.9, 128.9, 128.3 (dd, *J* = 11.7, 4.4 Hz), 126.5, 124.2 (d, *J* = 37.5 Hz), 122.3, 121.0, 110.6, 101.3, 44.9 (d, *J* = 3.4 Hz), 38.5, 34.7 (d, *J* = 66.8 Hz), 24.1, 21.2.

HRMS (ESI) calcd for $C_{32}H_{30}N_2O_2P^+[M+H]^+$: 505.2039; Found: 505.2030.

7-((diphenylphosphoryl)methyl)-3-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3c)



White solid, mp: 131-132 ºC. Yield: 65%.

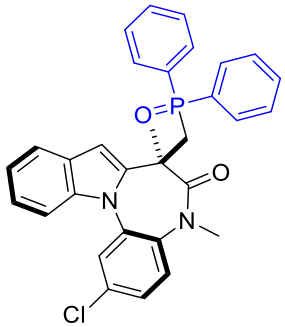
^{1}H NMR (500 MHz, Chloroform-d) δ 7.62–7.56 (m, 2H), 7.49–7.38 (m, 3H), 7.38–7.32 (m, 5H), 7.27 (d, *J* = 9.0 Hz, 1H), 7.25–7.18 (m, 3H), 7.18–7.13 (m, 1H), 7.05 (d, *J* = 2.9 Hz, 1H), 6.91 (dd, *J* = 9.0, 2.9 Hz, 1H), 6.49 (s, 1H), 3.87 (s, 3H), 3.24 (s, 3H), 2.58 (dd, *J* = 15.5, 13.4 Hz, 1H), 2.37 (dd, *J* = 15.6, 9.8 Hz, 1H), 1.94 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.72.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.7 (d, *J* = 7.5 Hz), 157.3, 143.2 (d, *J* = 9.4 Hz), 135.7, 134.0, 133.2 (d, *J* = 5.0 Hz), 132.9, 132.1, 131.7 (dd, *J* = 26.3, 2.8 Hz), 130.9 (d, *J* = 9.5 Hz), 130.8, 130.6 (d, *J* = 9.5 Hz), 129.0, 128.4 (dd, *J* = 14.8, 11.8 Hz), 125.1, 122.5, 121.2 (d, *J* = 13.9 Hz), 112.5, 110.6, 109.5, 101.9, 56.0, 44.8 (d, *J* = 3.3 Hz), 38.6, 34.7 (d, *J* = 66.9 Hz), 24.2.

HRMS (ESI) calcd for $C_{32}H_{30}N_2O_3P^+[M+H]^+$: 521.1989; Found: 521.1985.

3-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3d)



White solid, mp: 128-129 ºC. Yield: 70%.

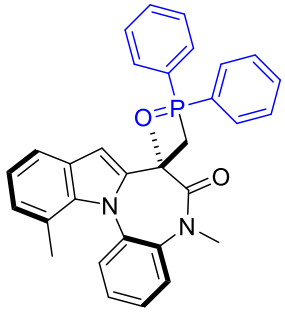
^{1}H NMR (500 MHz, Chloroform-d) δ 7.63–7.59 (m, 1H), 7.51–7.46 (m, 2H), 7.46–7.38 (m, 1H), 7.38–7.34 (m, 3H), 7.34–7.28 (m, 5H), 7.28–7.26 (m, 1H), 7.25–7.17 (m, 4H), 6.58 (d, *J* = 0.8 Hz, 1H), 3.30 (s, 3H), 2.63–2.49 (m, 1H), 2.35 (dd, *J* = 15.4, 8.8 Hz, 1H), 1.97 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.39.

^{13}C NMR (126 MHz, Chloroform-d) δ 169.2, 144.8, 140.8, 137.0 (d, *J* = 37.7 Hz), 136.0, 132.0, 129.6, 128.8, 128.0, 127.2, 126.2, 124.4 (d, *J* = 30.0 Hz), 122.9, 121.3 (d, *J* = 23.1 Hz), 110.7, 102.5, 59.1, 45.4, 38.7, 22.3 (d, *J* = 172.8 Hz).

HRMS (ESI) calcd for $C_{31}H_{27}ClN_2O_2P^+[M+H]^+$: 525.1493; Found: 525.1486.

7-((diphenylphosphoryl)methyl)-5,7,12-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3e)



White solid, mp: 206-207 ºC. Yield: 86%.

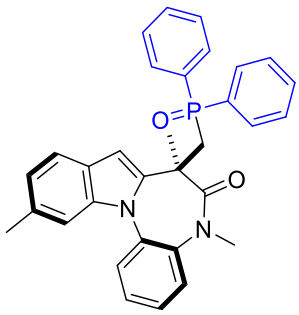
^{1}H NMR (500 MHz, Chloroform-d) δ 7.46–7.41 (m, 4H), 7.39–7.31 (m, 7H), 7.29–7.25 (m, 2H), 7.24–7.20 (m, 1H), 7.13–7.07 (m, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 6.92 (d, *J* = 8.6 Hz, 1H), 6.52 (s, 1H), 3.33 (s, 3H), 2.36 (dd, *J* = 15.6, 12.9 Hz, 1H), 2.20 (dd, *J* = 15.6, 10.2 Hz, 1H), 2.09 (s, 3H), 1.90 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.13.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.9 (d, *J* = 6.1 Hz), 146.0 (d, *J* = 10.1 Hz), 137.4, 135.7, 134.1, 133.6, 133.3 (d, *J* = 5.4 Hz), 132.5, 131.6 (dd, *J* = 8.2, 2.7 Hz), 131.0 (d, *J* = 9.4 Hz), 130.6 (d, *J* = 9.4 Hz), 130.1, 128.4 (dd, *J* = 11.7, 2.5 Hz), 128.3, 127.4, 126.8, 125.9, 125.1, 123.3, 121.7 (d, *J* = 38.4 Hz), 118.7, 103.2, 45.0 (d, *J* = 3.2 Hz), 37.8, 34.8 (d, *J* = 66.2 Hz), 24.6, 21.1.

HRMS (ESI) calcd for $C_{32}H_{30}N_2O_2P^+[M+H]^+$: 505.2039; Found: 505.2031.

7-((diphenylphosphoryl)methyl)-5,7,11-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3f)



White solid, mp: 270-271 ºC. Yield: 81%.

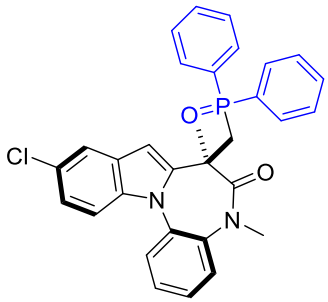
^{1}H NMR (500 MHz, Chloroform-d) δ 7.55–7.51 (m, 1H), 7.49–7.43 (m, 2H), 7.43–7.38 (m, 2H), 7.38–7.32 (m, 8H), 7.32–7.28 (m, 1H), 7.26–7.20 (m, 2H), 7.00 (dd, *J* = 8.1, 1.4 Hz, 1H), 6.43 (s, 1H), 3.27 (s, 3H), 2.56 (dd, *J* = 15.6, 13.4 Hz, 1H), 2.45 (s, 3H), 2.31 (dd, *J* = 15.5, 9.8 Hz, 1H), 1.93 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.58.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.8 (d, *J* = 7.2 Hz), 142.6 (d, *J* = 9.6 Hz), 137.4, 136.2, 134.0, 133.2, 132.9, 132.5 (d, *J* = 15.3 Hz), 132.1, 131.6 (dd, *J* = 18.6, 2.7 Hz), 130.9 (d, *J* = 9.2 Hz), 130.6 (d, *J* = 9.2 Hz), 128.5–128.1 (m), 126.8, 125.8, 124.5, 124.1, 122.9, 120.7, 110.5, 101.5, 44.9 (d, *J* = 3.3 Hz), 38.5, 34.8 (d, *J* = 66.6 Hz), 24.1, 22.0.

HRMS (ESI) calcd for $C_{32}H_{30}N_2O_2P^+$ $[M+H]^+$: 505.2039; Found: 505.2029.

10-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3g)



White solid, mp: 256-257 ºC. Yield: 85%.

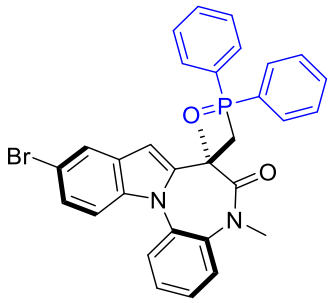
^{1}H NMR (500 MHz, Chloroform-d) δ 7.52 (d, *J* = 2.1 Hz, 1H), 7.43–7.37 (m, 5H), 7.36–7.27 (m, 8H), 7.23–7.15 (m, 2H), 7.12 (dd, *J* = 8.8, 2.1 Hz, 1H), 6.41 (s, 1H), 3.29 (s, 3H), 2.56–2.43 (m, 1H), 2.37–2.31 (m, 1H), 1.94 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.17.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.6 (d, *J* = 8.2 Hz), 144.4 (d, *J* = 8.9 Hz), 137.3, 134.2, 133.9, 133.1, 132.8, 132.0 (d, *J* = 9.5 Hz), 131.7 (dd, *J* = 23.9, 2.8 Hz), 130.9 (d, *J* = 9.4 Hz), 130.5 (d, *J* = 9.2 Hz), 130.0, 128.3 (dd, *J* = 21.5, 11.8 Hz), 127.2, 126.6, 125.8, 124.2 (d, *J* = 32.7 Hz), 122.6, 120.3, 111.7, 101.3, 44.9 (d, *J* = 3.4 Hz), 38.6, 34.5 (d, *J* = 66.7 Hz), 24.1.

HRMS (ESI) calcd for $C_{31}H_{27}ClN_2O_2P^+$ $[M+H]^+$: 525.1493; Found: 525.1486.

10-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3h)



White solid, mp: 235-236 ºC. Yield: 55%.

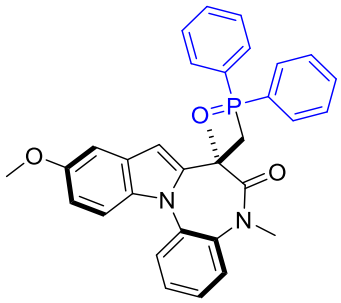
^{1}H NMR (500 MHz, Chloroform-d) δ 7.68 (d, *J* = 1.9 Hz, 1H), 7.49–7.44 (m, 1H), 7.44–7.41 (m, 1H), 7.41–7.37 (m, 3H), 7.36 (d, *J* = 4.3 Hz, 1H), 7.36–7.33 (m, 3H), 7.33–7.31 (m, 3H), 7.31–7.27 (m, 2H), 7.25–7.16 (m, 2H), 6.41 (s, 1H), 3.30 (s, 3H), 2.49 (dd, *J* = 15.5, 13.7 Hz, 1H), 2.32 (dd, *J* = 15.6, 9.5 Hz, 1H), 1.93 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.17.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.6 (d, *J* = 8.2 Hz), 144.3, 144.2, 137.3, 134.5, 133.9, 133.0 (d, *J* = 41.4 Hz), 132.0, 131.9, 131.7 (dd, *J* = 22.5, 2.7 Hz), 130.9 (d, *J* = 9.4 Hz), 130.6, 130.5 (d, *J* = 9.1 Hz), 128.3 (dd, *J* = 20.0, 11.8 Hz), 127.2, 125.8, 125.2, 124.2 (d, *J* = 30.8 Hz), 123.4, 114.2, 112.1, 101.2, 44.9 (d, *J* = 3.5 Hz), 38.6, 34.5 (d, *J* = 66.8 Hz), 24.1.

HRMS (ESI) calcd for $C_{31}H_{27}BrN_2O_2P^+$ $[M+H]^+$: 569.0988; Found: 569.0981.

7-((diphenylphosphoryl)methyl)-10-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3i)



White solid, mp: 188-189 ºC. Yield: 90%.

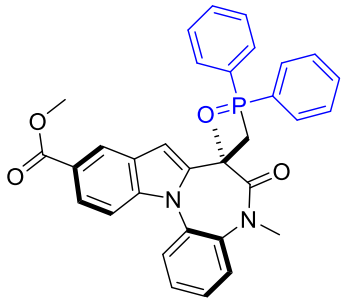
^{1}H NMR (500 MHz, Chloroform-d) δ 7.41 (d, *J* = 7.9 Hz, 1H), 7.38–7.33 (m, 2H), 7.32–7.21 (m, 11H), 7.18–7.11 (m, 2H), 6.95 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.34 (s, 1H), 3.21 (s, 3H), 2.48 (dd, *J* = 15.6, 13.4 Hz, 1H), 2.38 (s, 3H), 2.24 (dd, *J* = 15.6, 9.8 Hz, 1H), 1.88 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.47.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.8 (d, *J* = 7.2 Hz), 143.2 (d, *J* = 9.4 Hz), 137.2, 134.2, 134.0, 133.0 (d, *J* = 35.7 Hz), 132.5, 132.1, 131.6 (dd, *J* = 21.5, 2.7 Hz), 131.0 (d, *J* = 9.5 Hz), 130.7–130.4 (m), 129.2, 128.3 (t, *J* = 12.4 Hz), 126.6, 125.7, 124.3, 124.0 (d, *J* = 2.1 Hz), 120.7, 110.3, 101.3, 44.9 (d, *J* = 3.5 Hz), 38.6, 34.8 (d, *J* = 66.7 Hz), 24.1, 21.4.

HRMS (ESI) calcd for $C_{32}H_{30}N_2O_3P^+$ $[M+H]^+$: 521.1989; Found: 521.1980.

methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-10-carboxylate (3j)



White solid, mp: 270-271 ºC. Yield: 53%.

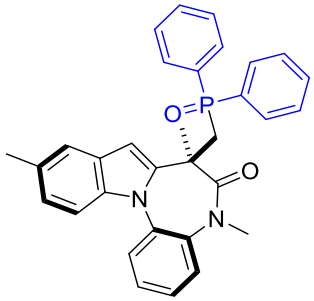
^{1}H NMR (500 MHz, Chloroform-d) δ 8.33 (d, *J* = 1.6 Hz, 1H), 7.89 (dd, *J* = 8.8, 1.7 Hz, 1H), 7.52 (d, *J* = 8.7 Hz, 1H), 7.46–7.39 (m, 4H), 7.38–7.27 (m, 8H), 7.23–7.12 (m, 2H), 6.56 (s, 1H), 3.94 (s, 3H), 3.32 (s, 3H), 2.51 (dd, *J* = 15.5, 13.9 Hz, 1H), 2.39–2.27 (m, 1H), 1.95 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.20.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.6 (d, *J* = 8.2 Hz), 167.8, 144.5 (d, *J* = 8.7 Hz), 138.2, 137.4, 133.9, 133.1, 132.7, 131.9, 131.7 (dd, *J* = 23.9, 2.6 Hz), 130.9 (d, *J* = 9.4 Hz), 130.5 (d, *J* = 9.1 Hz), 128.9, 128.8, 128.6–128.0 (m), 127.5, 125.9, 124.3 (d, *J* = 52.6 Hz), 123.8, 123.1, 110.4, 102.8, 52.0, 45.0 (d, *J* = 3.4 Hz), 38.6, 34.5 (d, *J* = 66.8 Hz), 24.1.

HRMS (ESI) calcd for $C_{33}H_{30}N_2O_4P^+$ $[M+H]^+$: 549.1938; Found: 549.1929.

7-((diphenylphosphoryl)methyl)-5,7,10-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3k)



White solid, mp: 247-248 ºC. Yield: 88%.

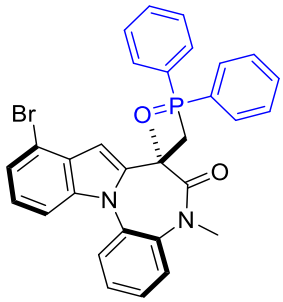
^{1}H NMR (500 MHz, Chloroform-d) δ 7.50–7.46 (m, 1H), 7.46–7.38 (m, 3H), 7.38–7.32 (m, 8H), 7.32–7.28 (m, 2H), 7.24–7.19 (m, 2H), 7.02 (dd, *J* = 8.4, 1.7 Hz, 1H), 6.41 (s, 1H), 3.27 (s, 3H), 2.55 (dd, *J* = 15.5, 13.4 Hz, 1H), 2.44 (s, 3H), 2.32 (dd, *J* = 15.5, 9.9 Hz, 1H), 1.95 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.64.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.8 (d, *J* = 7.4 Hz), 143.2 (d, *J* = 9.5 Hz), 137.2, 134.2, 133.9, 133.0 (d, *J* = 33.9 Hz), 132.5, 132.1, 131.6 (dd, *J* = 22.0, 2.7 Hz), 130.9 (d, *J* = 9.3 Hz), 130.6–130.5 (m), 129.2, 128.3 (dd, *J* = 13.6, 11.8 Hz), 126.7, 125.7, 124.3, 124.0 (d, *J* = 3.7 Hz), 120.7, 110.3, 101.3, 44.9 (d, *J* = 3.4 Hz), 38.5, 34.7 (d, *J* = 66.8 Hz), 24.1, 21.4.

HRMS (ESI) calcd for $C_{32}H_{30}N_2O_2P^+$$[M+H]^+$: 505.2039; Found: 505.2031.

9-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3l)



White solid, mp: 282-283 ºC. Yield: 52%.

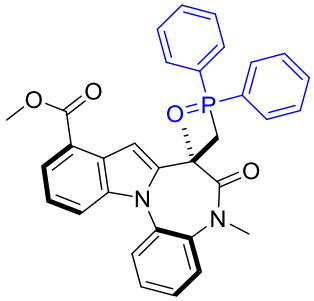
^{1}H NMR (500 MHz, Chloroform-d) δ 7.53 (d, *J* = 7.8 Hz, 1H), 7.51–7.46 (m, 1H), 7.46–7.41 (m, 1H), 7.39–7.36 (m, 4H), 7.35–7.27 (m, 6H), 7.23–7.15 (m, 2H), 7.14–7.08 (m, 1H), 6.96 (d, *J* = 7.1 Hz, 1H), 6.46 (s, 1H), 3.28 (s, 3H), 2.59–2.53 (m, 1H), 2.35 (dd, *J* = 15.5, 9.6 Hz, 1H), 2.00 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.53.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.8 (d, *J* = 7.8 Hz), 142.4 (d, *J* = 8.9 Hz), 137.3, 135.5, 133.9, 133.0 (d, *J* = 45.8 Hz), 132.6, 132.0, 131.6 (dd, *J* = 34.6, 2.9 Hz), 131.0–130.2 (m), 128.7, 128.3 (dd, *J* = 24.1, 11.7 Hz), 126.8, 125.8, 124.2 (d, *J* = 57.9 Hz), 122.6, 121.3, 108.3, 100.3, 44.9 (d, *J* = 3.4 Hz), 38.5, 34.7 (d, *J* = 66.8 Hz), 24.1.

HRMS (ESI) calcd for $C_{31}H_{27}BrN_2O_2P^+$[M+H]$^+$: 569.0988; Found: 569.0980

Methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-9-carboxylate (3m)



White solid, mp: 286-287 ºC. Yield: 58%.

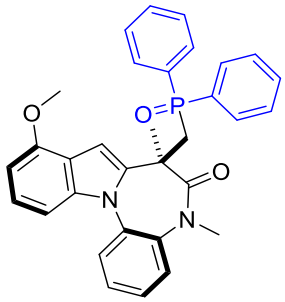
^{1}H NMR (500 MHz, Chloroform-d) δ 7.93 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.73 (d, *J* = 8.2 Hz, 1H), 7.48–7.37 (m, 6H), 7.35–7.27 (m, 6H), 7.24–7.20 (m, 3H), 7.13 (s, 1H), 3.98 (s, 3H), 3.31 (s, 3H), 2.59–2.47 (m, 1H), 2.38–2.25 (m, 1H), 1.96 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.98.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.6 (d, *J* = 8.2 Hz), 167.8, 144.5 (d, *J* = 8.7 Hz), 138.2, 137.5, 133.9, 133.1, 132.7, 132.0, 131.9–131.5 (m), 131.6, 131.6, 130.9 (dd, *J* = 9.7, 5.7 Hz), 130.5 (d, *J* = 9.1 Hz), 128.8 (d, *J* = 12.3 Hz), 128.7–128.0 (m), 127.5, 125.9, 124.3 (d, *J* = 52.6 Hz), 123.8, 123.2, 110.4, 102.9, 52.0, 45.0 (d, *J* = 3.4 Hz), 38.6, 34.5 (d, *J* = 66.8 Hz), 24.1.

HRMS (ESI) calcd for $C_{33}H_{30}N_2O_4P^+$ [M+H]$^+$: 549.1938, Found: 549.1932.

7-((diphenylphosphoryl)methyl)-9-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3n)



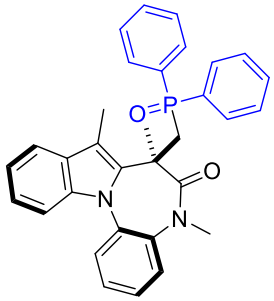
White solid, mp: 208-209 ºC. Yield: 80%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.53 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.44–7.37 (m, 3H), 7.37–7.31 (m, 6H), 7.31–7.27 (m, 2H), 7.25–7.20 (m, 2H), 7.18–7.09 (m, 2H), 6.62–6.55 (m, 2H), 3.94 (s, 3H), 3.26 (s, 3H), 2.54 (dd, *J* = 15.5, 13.4 Hz, 1H), 2.36–2.27 (m, 1H), 1.95 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 26.33.

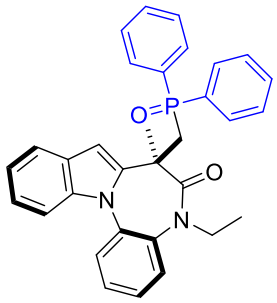
^{13}C NMR (126 MHz, Chloroform-d) δ 170.7 (d, *J* = 7.0 Hz), 153.4, 141.8 (d, *J* = 9.8 Hz), 137.3 (d, *J* = 33.2 Hz), 134.0, 133.1 (d, *J* = 29.2 Hz), 132.5, 132.2, 131.6 (dd, *J* = 23.4, 2.8 Hz), 130.8 (dd, *J* = 41.6, 9.3 Hz), 128.3 (t, *J* = 11.3 Hz), 126.9, 125.7, 124.3 (d, *J* = 57.7 Hz), 123.4, 119.6, 104.0, 101.0, 98.9, 55.5, 44.8 (d, *J* = 3.2 Hz), 38.5, 34.8 (d, *J* = 66.6 Hz), 24.1.
HRMS (ESI) calcd for $C_{32}H_{30}N_2O_3P^+$ $[M+H]^+$: 521.1989; Found: 521.1982.

7-((diphenylphosphoryl)methyl)-5,7,8-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3o)



White solid, mp: 285-286 ºC. Yield: 69%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.58–7.50 (m, 1H), 7.45–7.40 (m, 2H), 7.38–7.26 (m, 10H), 7.26–7.23 (m, 1H), 7.20–7.14 (m, 2H), 7.14–7.09 (m, 2H), 3.33 (s, 3H), 2.54–2.46 (m, 2H), 2.42 (s, 3H), 2.17–2.15 (m, 3H).
^{31}P NMR (202 MHz, Chloroform-d) δ 26.20.
^{13}C NMR (126 MHz, Chloroform-d) δ 171.0 (d, *J* = 9.2 Hz), 137.5, 136.4 (d, *J* = 7.9 Hz), 135.0, 134.3, 133.5, 132.9, 132.9, 132.2, 131.6 (d, *J* = 2.6 Hz), 131.4–131.1 (m), 130.6 (dd, *J* = 57.0, 9.3 Hz), 128.2 (dd, *J* = 40.2, 11.7 Hz), 126.7, 125.4 (d, *J* = 50.9 Hz), 123.4, 122.7, 120.6, 119.0, 110.8, 110.4, 47.3 (d, *J* = 3.6 Hz), 38.4, 35.9 (d, *J* = 66.7 Hz), 25.5, 11.0.
HRMS (ESI) calcd for $C_{32}H_{31}N_2O_2P^+$ $[M+H]^+$: 505.2039; Found: 505.2030.

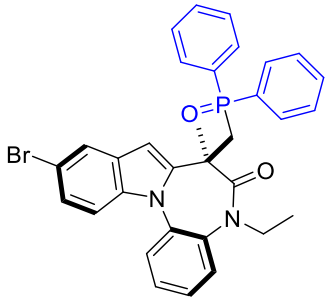
7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3p)



White solid, mp: 184-185 ºC. Yield: 63%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.59–7.55 (m, 1H), 7.55–7.50 (m, 1H), 7.48–7.39 (m, 3H), 7.39–7.27 (m, 9H), 7.22–7.10 (m, 4H), 6.47 (s, 1H), 4.14–3.96 (m, 1H), 3.74–3.60 (m, 1H), 2.50 (dd, *J* = 15.5, 14.0 Hz, 1H), 2.39 (dd, *J* = 15.5, 9.5 Hz, 1H), 1.99 (s, 3H), 1.07 (t, *J* = 7.1 Hz, 3H).
^{31}P NMR (202 MHz, Chloroform-d) δ 26.32.

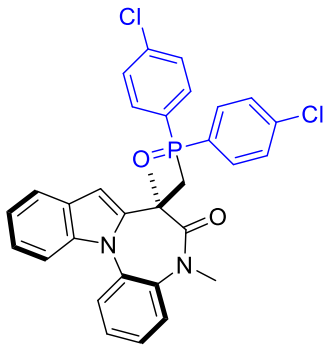
^{13}C NMR (126 MHz, Chloroform-d) δ 169.9 (d, *J* = 8.5 Hz), 143.1 (d, *J* = 8.6 Hz), 136.2, 135.8, 134.2, 133.4 (d, *J* = 9.0 Hz), 133.0, 132.2, 131.5 (dd, *J* = 34.9, 2.8 Hz), 130.9 (d, *J* = 9.5 Hz), 130.5 (d, *J* = 9.1 Hz), 129.1, 128.3 (dd, *J* = 31.7, 11.8 Hz), 126.9, 126.1, 124.5 (d, *J* = 20.8 Hz), 122.4, 121.1 (d, *J* = 9.4 Hz), 110.6, 102.0, 46.1, 45.1 (d, *J* = 3.6 Hz), 34.5 (d, *J* = 67.0 Hz), 24.1 (d, *J* = 1.9 Hz), 13.4.
HRMS (ESI) calcd for $C_{32}H_{30}N_2O_2P^+$ $[M+H]^+$: 505.2039; Found: 505.2030.

10-bromo-7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3q)



White solid, mp: 125-126 ºC. Yield: 75%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.67 (d, *J* = 1.9 Hz, 1H), 7.47–7.27 (m, 13H), 7.24 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.19–7.12 (m, 2H), 6.38 (s, 1H), 4.16–3.96 (m, 1H), 3.76–3.54 (m, 1H), 2.48–2.34 (m, 2H), 1.95 (s, 3H), 1.05 (t, *J* = 7.1 Hz, 3H).
^{31}P NMR (202 MHz, Chloroform-d) δ 26.13.
^{13}C NMR (126 MHz, Chloroform-d) δ 169.7 (d, *J* = 9.0 Hz), 144.2 (d, *J* = 8.1 Hz), 136.2, 134.5, 134.1, 133.3, 132.9 (d, *J* = 7.1 Hz), 132.1, 131.6 (dd, *J* = 30.9, 2.7 Hz), 131.0–130.7 (m), 130.4 (d, *J* = 9.0 Hz), 128.4 (d, *J* = 11.7 Hz), 128.2 (d, *J* = 11.8 Hz), 127.3, 126.3, 125.2, 124.5 (d, *J* = 2.3 Hz), 123.4, 114.1, 112.1, 101.4, 46.1, 45.2 (d, *J* = 3.6 Hz), 34.2 (d, *J* = 67.0 Hz), 24.0, 13.4.
HRMS (ESI) calcd for $C_{32}H_{29}BrN_2O_2P^+$ $[M+H]^+$: 583.1145; Found: 583.1139.

7-((bis(4-chlorophenyl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3r)

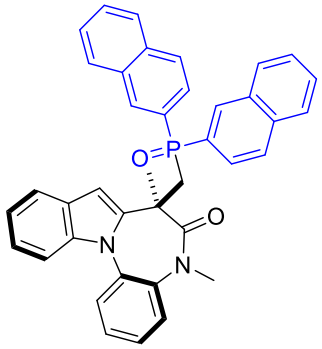


White solid, mp: 149-150 ºC. Yield: 58%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.60–7.53 (m, 3H), 7.42–7.39 (m, 2H), 7.38–7.26 (m, 5H), 7.23–7.15 (m, 6H), 6.44 (s, 1H), 3.31 (s, 3H), 2.54–2.44 (m, 1H), 2.32 (dd, *J* = 15.5, 9.3 Hz, 1H), 1.93 (s, 3H).
^{31}P NMR (202 MHz, Chloroform-d) δ 25.44.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.5 (d, *J* = 8.4 Hz), 142.5 (d, *J* = 8.7 Hz), 138.5 (dd, *J* = 11.3, 3.3 Hz), 137.3, 135.7, 132.4–132.1 (m), 131.8 (d, *J* = 10.0 Hz), 131.3, 130.9, 130.1, 129.4–128.2 (m), 127.0, 125.9, 124.2 (d, *J* = 29.8 Hz), 122.7, 121.3 (d, *J* = 39.2 Hz), 110.6, 102.0, 44.8 (d, *J* = 3.5 Hz), 38.6, 34.5 (d, *J* = 67.9 Hz), 24.1.

HRMS (ESI) calcd for $C_{31}H_{26}CI_2N_2O_2P^+$ $[M+H]^+$: 559.1103; Found: 559.1099.

7-((di(naphthalen-2-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3s)



White solid, mp: 166-167 ºC. Yield: 63%.

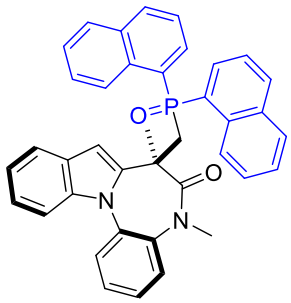
^{1}H NMR (500 MHz, Chloroform-d) δ 8.11 (d, *J* = 13.5 Hz, 1H), 7.95 (d, *J* = 13.2 Hz, 1H), 7.84–7.77 (m, 3H), 7.73–7.65 (m, 2H), 7.59–7.46 (m, 7H), 7.42–7.35 (m, 3H), 7.34–7.27 (m, 2H), 7.25–7.20 (m, 1H), 7.19–7.10 (m, 2H), 6.48 (s, 1H), 3.28 (s, 3H), 2.76 (dd, *J* = 15.5, 13.9 Hz, 1H), 2.56 (dd, *J* = 15.5, 9.2 Hz, 1H), 2.06 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 27.11.

^{13}C NMR (126 MHz, Chloroform-d) δ 170.9 (d, *J* = 8.4 Hz), 142.9 (d, *J* = 8.7 Hz), 137.3, 135.8, 134.5 (dd, *J* = 14.5, 2.3 Hz), 133.2 (d, *J* = 8.6 Hz), 132.5–132.1 (m), 131.1, 130.3, 129.9, 129.2, 129.0, 128.8 (d, *J* = 1.7 Hz), 128.2 (t, *J* = 13.3 Hz), 128.0 (d, *J* = 11.8 Hz), 127.7 (d, *J* = 17.8 Hz), 127.0, 126.9 (d, *J* = 5.0 Hz), 125.8, 125.5 (dd, *J* = 13.6, 10.4 Hz), 124.2 (d, *J* = 40.3 Hz), 122.5, 121.1 (d, *J* = 26.2 Hz), 110.6, 102.0, 45.0 (d, *J* = 3.4 Hz), 38.6, 34.4 (d, *J* = 67.2 Hz), 24.2.

HRMS (ESI) calcd for $C_{39}H_{32}N_2O_2P^+$ $[M+H]^+$: 591.2196; Found: 591.2187.

7-((di(naphthalen-1-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3t)



White solid, mp: 197-198 ºC. Yield: 70%.

^{1}H NMR (500 MHz, Chloroform-d) δ 8.28 (d, *J* = 8.6 Hz, 1H), 8.07 (d, *J* = 8.6 Hz, 1H), 7.95–7.87 (m, 2H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.78–7.71 (m, 2H), 7.61–7.53 (m, 2H), 7.53–7.48 (m, 1H), 7.43–7.38 (m,

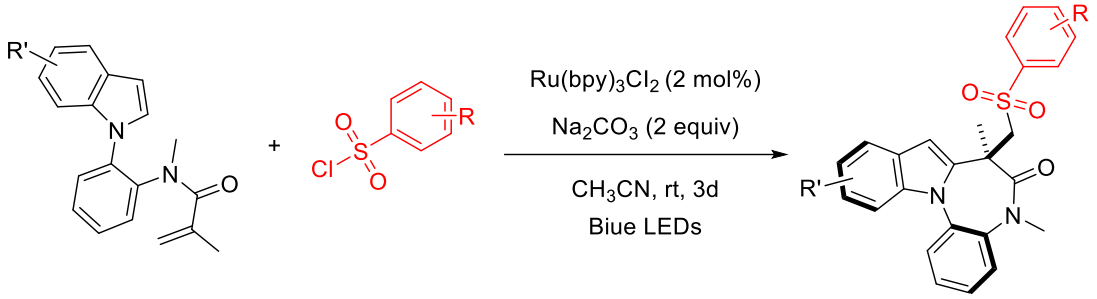
1H), 7.38–7.28 (m, 4H), 7.25–7.20 (m, 1H), 7.20–7.13 (m, 4H), 7.09–6.99 (m, 2H), 6.48 (s, 1H), 3.31 (s, 3H), 3.12 (dd, *J* = 15.1, 13.8 Hz, 1H), 2.75 (dd, *J* = 15.1, 9.1 Hz, 1H), 1.93 (s, 3H).

^{31}P NMR (202 MHz, Chloroform-d) δ 27.31.

^{13}C NMR (126 MHz, Chloroform-d) δ 171.0 (d, *J* = 7.8 Hz), 143.2 (d, *J* = 9.2 Hz), 137.0, 135.8, 133.8 (dd, *J* = 23.6, 9.1 Hz), 133.1 (d, *J* = 3.1 Hz), 133.0–132.7 (m), 132.5 (d, *J* = 9.1 Hz), 132.1, 131.6, 130.8 (d, *J* = 12.2 Hz), 130.3 (d, *J* = 9.3 Hz), 130.0, 128.9 (d, *J* = 15.6 Hz), 127.1 (d, *J* = 23.0 Hz), 126.7, 126.3 (d, *J* = 5.0 Hz), 126.0, 125.5 (d, *J* = 4.8 Hz), 125.4, 124.5 (d, *J* = 13.4 Hz), 124.1 (d, *J* = 13.2 Hz), 123.9 (d, *J* = 5.8 Hz), 122.4, 121.1 (d, *J* = 8.0 Hz), 110.7, 102.1, 45.2 (d, *J* = 2.9 Hz), 38.7, 33.6 (d, *J* = 68.4 Hz), 24.0.

HRMS (ESI) calcd for $C_{39}H_{32}N_2O_2P^+$ $[M+H]^+$: 591.2196; Found: 591.2189.

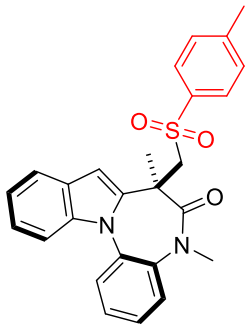
4 General procedure for photocatalyzed sulfonation cyclization reaction



1 **4** **5**

In the glove box filled with high-purity argon, a 10 mL Young tube was charged with N-Methyl-aryl acrylamide (0.2 mmol, 1 equiv.), Tosyl chloride (0.4 mmol, 2 equiv.), $Ru(bpy)_3Cl_2$ (2.6 mg, 2 mol%), Na_2CO_3 (46.4 mg, 2 equiv), and 4 mL MeCN. Then, the tube was removed from the glove box. The reaction mixture was stirred at at room temperature for 3d under blue LEDs. Upon completion, proper amount of silica gel was added to the reaction mixture. the crude product was purified by column chromatography, eluting with PE/EA (5:1) to afford the desired product.

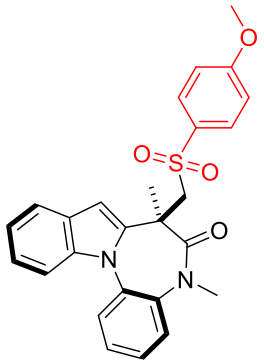
5,7-dimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5a)



White solid, mp: 199-200 ºC. Yield: 91%.

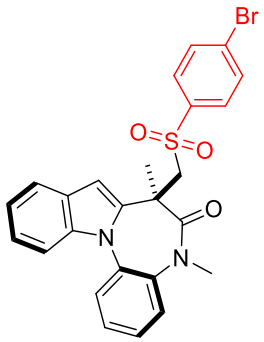
^{1}H NMR (500 MHz, Chloroform-d) δ 7.64–7.60 (m, 1H), 7.57–7.52 (m, 2H), 7.45–7.42 (m, 2H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.35–7.31 (m, 1H), 7.24–7.17 (m, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 6.57 (d, *J* = 0.8 Hz, 1H), 3.36 (s, 3H), 3.13 (d, *J* = 14.8 Hz, 1H), 3.04 (d, *J* = 14.8 Hz, 1H), 2.34 (s, 3H), 2.04 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.8, 170.7, 142.8, 142.7, 135.8, 135.6, 134.1, 133.3, 133.2, 132.6, 131.9, 131.9, 131.8, 131.6, 131.6, 131.0, 130.9, 130.9, 130.4, 130.3, 129.0, 128.6, 128.5, 128.4, 128.3, 126.8, 125.0, 124.0, 122.9, 121.6, 121.3, 110.4, 102.6, 44.9, 44.9, 38.7, 35.4, 34.9, 24.3.
HRMS (ESI) calcd for $C_{26}H_{25}N_2O_3S^+$ $[M+H]^+$:445.1580;Found:445.1573.

7-(((4-methoxyphenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5b)



White solid, mp: 190-191 ºC. Yield: 89%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.63 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.48–7.43 (m, 2H), 7.41 (d, *J* = 8.6 Hz, 2H), 7.37–7.29 (m, 1H), 7.25–7.16 (m, 2H), 6.78 (d, *J* = 8.5 Hz, 2H), 6.60 (s, 1H), 3.77 (s, 3H), 3.37 (s, 3H), 3.15 (d, *J* = 14.8 Hz, 1H), 3.07 (d, *J* = 14.8 Hz, 1H), 2.09 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.3, 163.7, 140.7, 136.8, 136.0, 131.9, 131.5, 130.3, 128.8, 127.2, 126.3, 124.5, 124.2, 122.8, 121.4, 121.2, 114.1, 110.8, 102.6, 59.2, 55.7, 45.5, 38.7, 22.9.
HRMS (ESI) calcd for $C_{26}H_{25}N_2O_4S^+$ $[M+H]^+$:461.1530; Found: 460.1523.

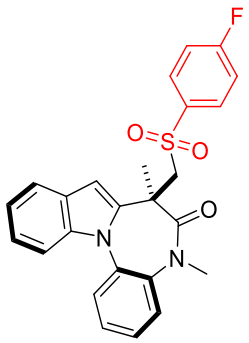
7-(((4-bromophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5c)



White solid, mp: 234-235 ºC. Yield: 83%.

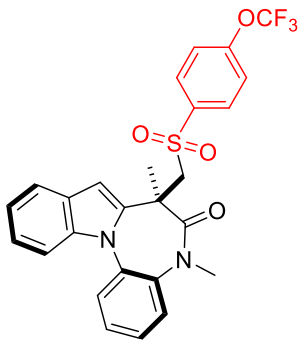
^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 7.3 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.54–7.47 (m, 3H), 7.47–7.41 (m, 2H), 7.38–7.30 (m, 3H), 7.27–7.13 (m, 2H), 6.62 (s, 1H), 3.38 (s, 3H), 3.15 (d, *J* = 14.8 Hz, 1H), 3.08 (d, *J* = 14.8 Hz, 1H), 2.08 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.0, 140.4, 138.9, 136.7, 136.0, 132.3, 131.9, 129.6, 129.2, 128.7, 127.2, 126.3, 124.5, 124.2, 123.1, 121.5, 121.3, 110.7, 102.8, 59.2, 45.4, 38.8, 23.0.
HRMS (ESI) calcd for $C_{25}H_{23}BrN_2O_3S^+$ $[M+H]^+$: 509.0529; Found: 509.0523.

7-(((4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5d)



White solid, mp: 229-230 ºC. Yield: 77%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J* = 8.2 Hz, 1H), 7.54–7.49 (m, 3H), 7.45 (d, *J* = 4.0 Hz, 2H), 7.36–7.32 (m, 1H), 7.25–7.18 (m, 2H), 7.04 (t, *J* = 8.5 Hz, 2H), 6.62 (s, 1H), 3.39 (s, 3H), 3.16 (d, *J* = 14.8 Hz, 1H), 3.08 (d, *J* = 14.8 Hz, 1H), 2.08 (s, 3H).
^{19}F NMR (471 MHz, Chloroform-d) δ -102.98.
^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.1, 165.8 (d, *J* = 256.9 Hz), 140.5, 136.8, 136.1 (d, *J* = 3.1 Hz), 136.0, 132.0, 131.0 (d, *J* = 9.6 Hz), 128.7, 127.2, 126.3, 124.5, 124.2, 123.0, 121.5, 121.2, 116.4, 116.2, 110.7, 102.7, 77.3, 77.1, 76.8, 59.3, 45.4, 38.7, 23.0.
HRMS (ESI) calcd for $C_{25}H_{22}FN_2O_3S^+$$[M+H]^+$: 449.1330; Found: 449.1323.

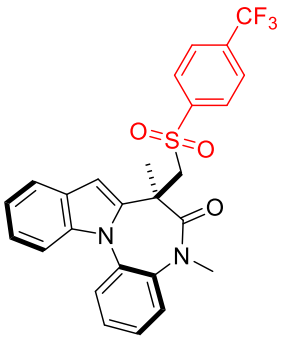
5,7-dimethyl-7-(((4-(trifluoromethoxy)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5e)



White solid, mp: 207-208 ºC .Yield: 84%.

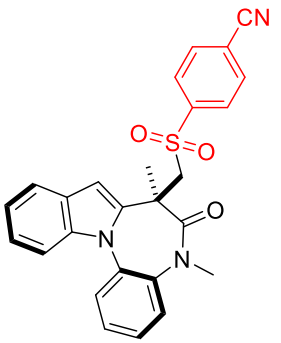
^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.47–7.39 (m, 3H), 7.36–7.28 (m, 1H), 7.23 (dd, *J* = 12.2, 7.8 Hz, 2H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.65 (s, 1H), 3.38 (s, 3H), 3.19 (d, *J* = 14.9 Hz, 1H), 3.13 (d, *J* = 14.9 Hz, 1H), 2.12 (s, 3H).
^{19}F NMR (471 MHz, Chloroform-d) δ -57.62.
^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.0, 152.9 (d, *J* = 2.0 Hz), 140.3, 138.2, 136.6, 135.9, 131.9, 130.5, 128.7, 127.2, 126.3, 124.4, 124.1, 123.1, 121.4 (d, J = 35.6 Hz), 120.8, 110.7, 102.8, 59.3, 45.4, 38.8, 23.0.
HRMS (ESI) calcd. for $C_{26}H_{22}F_3N_2O_4S^+$ $[M+H]^+$:515.1247; Found: 515.1239.

5,7-dimethyl-7-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5f)



White solid, mp: 214-215 ºC. Yield: 83%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.67–7.62 (m, 1H), 7.60 (s, 4H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.48–7.41 (m, 3H), 7.37–7.30 (m, 1H), 7.27–7.17 (m, 2H), 6.63 (s, 1H), 3.39 (s, 3H), 3.20 (d, *J* = 14.8 Hz, 1H), 3.14 (d, *J* = 14.9 Hz, 1H), 2.11 (s, 3H).
^{19}F NMR (471 MHz, Chloroform-d) δ -63.15.
^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.9, 143.3, 140.2, 136.7, 135.9, 135.4, 135.2, 131.9, 128.7, 128.7, 127.3, 126.4, 126.1 (q, *J* = 3.7 Hz)., 124.4, 124.2, 123.1, 121.6, 121.3, 110.8, 102.9, 59.1, 45.4, 38.8, 23.1.
HRMS (ESI) calcd for $C_{26}H_{22}F_3N_2O_3S^+$ $[M+H]^+$:499.1298; Found: 499.1293.

4-(((5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-7-yl)methyl)sulfonyl)benzonitrile (5g)



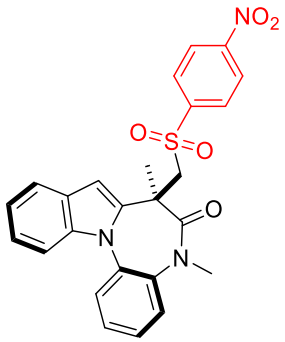
White solid, mp: 237-238 ºC. Yield:76%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.66–7.54 (m, 6H), 7.50–7.43 (m, 3H), 7.38–7.30 (m, 1H), 7.28–7.16 (m, 2H), 6.62 (s, 1H), 3.39 (s, 3H), 3.18 (d, *J* = 14.8 Hz, 1H), 3.12 (d, *J* = 14.8 Hz, 1H), 2.08 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.8, 143.9, 139.9, 136.7, 135.9, 132.9, 132.7, 131.9, 128.9, 128.8, 128.6, 127.3, 126.4, 124.4, 124.2, 123.2, 121.7, 121.3, 117.4, 116.9, 110.7, 103.0, 59.1, 45.3, 38.8, 23.1.

HRMS (ESI) calcd for $C_{26}H_{22}N_3O_3S^+$ $[M+H]^+$: 456.1376; Found: 456.1368.

5,7-dimethyl-7-(((4-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5h)



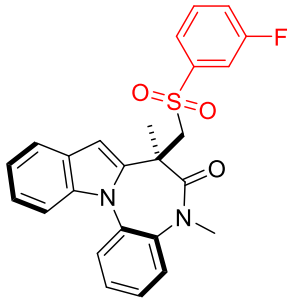
White solid, mp: 229-230 ºC. Yield:86%.

^{1}H NMR (500 MHz, Chloroform-d) δ 8.16 (d, *J* = 8.8 Hz, 2H), 7.67 (d, *J* = 8.8 Hz, 2H), 7.63 (d, *J* = 7.0 Hz, 1H), 7.54 (dd, *J* = 18.4, 8.2 Hz, 2H), 7.50–7.46 (m, 2H), 7.40–7.33 (m, 1H), 7.25–7.16 (m, 2H), 6.60 (s, 1H), 3.40 (s, 3H), 3.20 (d, *J* = 14.8 Hz, 1H), 3.15 (d, *J* = 14.8 Hz, 1H), 2.09 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.8, 150.6, 145.3, 139.9, 136.7, 135.9, 131.9, 129.5, 128.6, 127.4, 126.5, 124.4, 124.3, 124.2, 124.1, 123.2, 121.7, 121.3, 110.7, 103.0, 59.0, 45.3, 38.8, 23.1.

HRMS (ESI) calcd for $C_{25}H_{22}N_3O_5S^+$ $[M+H]^+$: 476.1275; Found: 476.1271.

7-(((3-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5i)



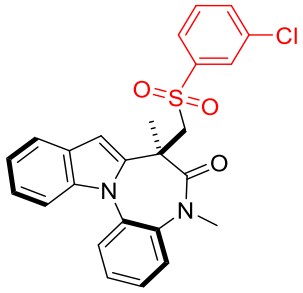
White solid, mp: 191-192 ºC. Yield:84%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.64 (d, *J* = 7.1 Hz, 1H), 7.54 (dd, *J* = 20.9, 7.8 Hz, 2H), 7.51–7.43 (m, 2H), 7.39–7.28 (m, 3H), 7.26–7.12 (m, 4H), 6.63 (s, 1H), 3.39 (s, 3H), 3.17 (d, *J* = 14.8 Hz, 1H), 3.10 (d, *J* = 14.8 Hz, 1H), 2.11 (s, 3H).

^{19}F NMR (471 MHz, Chloroform-d) δ -109.15.

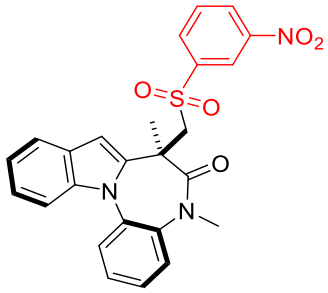
^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.0, 162.2 (d, *J* = 252.6 Hz), 140.4, 136.3 (d, *J* = 95.8 Hz), 132.0, 130.9 (d, *J* = 7.6 Hz), 128.7, 127.3, 126.4, 124.5, 124.2, 123.9 (d, *J* = 3.4 Hz), 123.0, 121.5, 121.3, 121.1, 121.0, 115.4, 115.2, 110.8, 102.7, 59.1, 45.4, 38.8, 23.0.
HRMS (ESI) calcd for $C_{25}H_{22}FN_2O_3S^+$ $[M+H]^+$: 449.1330; Found: 449.1335.

7-(((3-chlorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5j)



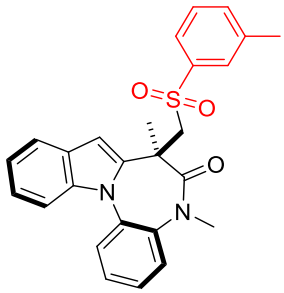
White solid, mp: 180-181 ºC. Yield: 82%.
^{1}H NMR (500 MHz, Chloroform-d) δ 7.64 (d, *J* = 7.8 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.52–7.41 (m, 4H), 7.42–7.32 (m, 3H), 7.27–7.16 (m, 3H), 6.63 (s, 1H), 3.37 (s, 3H), 3.17 (d, *J* = 14.8 Hz, 1H), 3.11 (d, *J* = 14.8 Hz, 1H), 2.14 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.0, 141.5, 140.3, 136.6, 135.9, 135.3, 133.8, 131.9, 130.3, 128.7, 128.1, 127.4, 126.4, 126.3, 124.5, 124.1, 123.0, 121.5, 121.3, 110.7, 102.8, 59.1, 45.4, 38.8, 23.0.
HRMS (ESI) calcd for $C_{25}H_{22}ClN_2O_3S^+$ $[M+H]^+$: 465.1034; Found: 465.1028.

5,7-dimethyl-7-(((3-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5k)



White solid, mp: 232-233 ºC. Yield: 79%.
^{1}H NMR (500 MHz, Chloroform-d) δ 8.31 (d, *J* = 8.1 Hz, 1H), 8.22–8.16 (m, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.62 (d, *J* = 7.0 Hz, 1H), 7.57–7.46 (m, 4H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.37–7.29 (m, 1H), 7.26–7.16 (m, 2H), 6.62 (s, 1H), 3.40 (s, 3H), 3.24–3.12 (m, 2H), 2.15 (s, 3H).
^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.8, 148.0, 141.7, 139.7, 136.6, 135.8, 133.7, 131.8, 130.3, 128.6, 128.1, 127.6, 126.4, 124.4, 124.1, 123.4, 123.2, 121.7, 121.3, 110.7, 103.1, 58.9, 45.3, 38.8, 22.9.
HRMS (ESI) calcd for $C_{25}H_{22}N_3O_5S^+$ $[M+H]^+$: 476.1275; Found: 476.1271.

5,7-dimethyl-7-((m-tolylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5l)



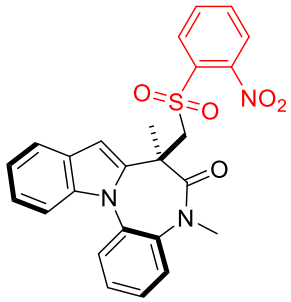
White solid, mp: 194-195 ºC. Yield:81%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 6.8 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.48–7.37 (m, 2H), 7.36–7.27 (m, 4H), 7.25–7.12 (m, 4H), 6.65 (s, 1H), 3.37 (s, 3H), 3.17 (d, *J* = 14.9 Hz, 1H), 3.11 (d, *J* = 14.9 Hz, 1H), 2.16 (d, *J* = 13.7 Hz, 6H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.2, 140.6, 139.8, 139.4, 136.7, 135.9, 134.4, 131.8, 128.9, 128.8, 128.4, 127.1, 126.1, 125.2, 124.5, 124.1, 122.9, 121.4, 121.3, 110.7, 102.7, 59.1, 45.5, 38.8, 23.0, 21.0.

HRMS (ESI) calcd for $C_{26}H_{25}N_2O_3S^+$ $[M+H]^+$: 445.1580; Found: 445.1572.

5,7-dimethyl-7-(((2-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5m)



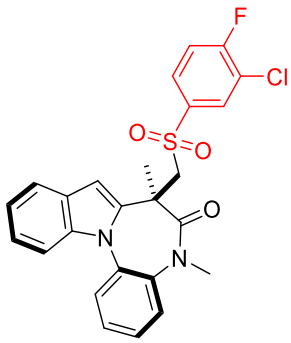
White solid, mp: 146-147 ºC. Yield: 91%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.70–7.65 (m, 3H), 7.57–7.49 (m, 3H), 7.40–7.36 (m, 2H), 7.25–7.17 (m, 4H), 6.70 (s, 1H), 3.99 (d, *J* = 15.2 Hz, 1H), 3.47 (d, *J* = 15.2 Hz, 1H), 3.43–3.39 (m, 3H), 2.12 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.1, 149.0, 140.2, 136.4, 135.8, 134.8, 134.0, 132.5, 132.1, 131.6, 130.5, 128.7, 127.5, 126.2, 124.8, 124.1, 123.1, 121.5, 121.3, 110.9, 103.2, 59.9, 45.7, 39.0, 23.4.

HRMS (ESI) calcd for $C_{25}H_{22}N_3O_5S^+$ $[M+H]^+$: 476.1275; Found: 476.1272

7-(((3-chloro-4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5n)



White solid, mp: 256-257 ºC. Yield: 87%

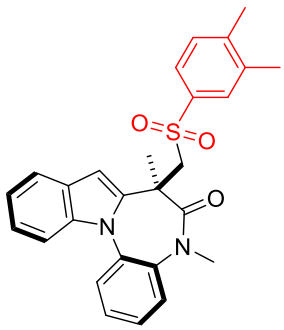
^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 7.1 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.52–7.43 (m, 4H), 7.44–7.37 (m, 1H), 7.40–7.33 (m, 1H), 7.27–7.17 (m, 2H), 7.12–7.01 (m, 1H), 6.63 (s, 1H), 3.39 (s, 3H), 3.17 (d, *J* = 14.8 Hz, 1H), 3.11 (d, *J* = 14.8 Hz, 1H), 2.12 (s, 3H).

^{19}F NMR (471 MHz, Chloroform-d) δ -105.16.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.9, δ 161.2 (d, *J* = 259.2 Hz), 140.1, 136.8 (d, *J* = 4.0 Hz), 136.7, 135.9, 131.9, 131.1, 128.8 (d, *J* = 8.8 Hz), 127.4, 126.4, 124.5, 124.1, 123.1, 122.6, 122.4, 121.6, 121.3, 117.2 (d, *J* = 22.4 Hz), 110.7, 102.9, 59.2, 45.4, 38.8, 23.0.

HRMS (ESI) calcd for $C_{25}H_{21}ClFN_2O_3S^+$ $[M+H]^+$: 483.0940; Found: 483.0936.

7-(((3,4-dimethylphenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5o)



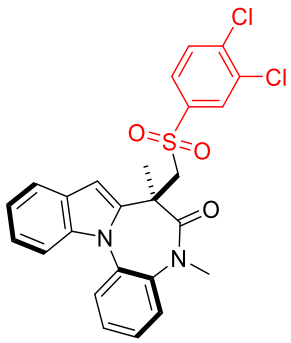
White solid, mp: 211-212 ºC. Yield: 68%

^{1}H NMR (500 MHz, Chloroform-d) δ 7.64 (d, *J* = 7.3 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.47–7.41 (m, 2H), 7.41–7.37 (m, 1H), 7.34–7.27 (m, 1H), 7.25–7.15 (m, 3H), 7.15–7.06 (m, 2H), 6.60 (s, 1H), 3.37 (s, 3H), 3.14 (d, *J* = 14.9 Hz, 1H), 3.08 (d, *J* = 14.8 Hz, 1H), 2.23 (s, 3H), 2.12–2.08 (m, 6H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.3, 143.4, 140.6, 137.9, 137.1, 136.8, 135.9, 131.9, 130.0, 128.8, 128.7, 127.1, 126.1, 125.6, 124.5, 124.1, 122.8, 121.4, 121.2, 110.7, 102.7, 59.0, 45.5, 38.7, 22.9, 19.9, 19.5.

HRMS (ESI) calcd for $C_{27}H_{27}N_2O_3S^+$ $[M+H]^+$: 459.1737; Found: 459.1732.

7-(((3,4-dichlorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5p)



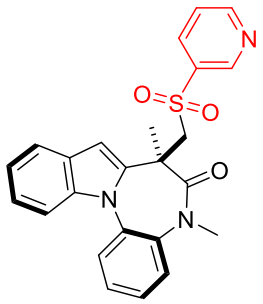
White solid, mp: 248-249 ºC. Yield: 91%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.65 (d, *J* = 7.1 Hz, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.52–7.42 (m, 4H), 7.41–7.33 (m, 2H), 7.34–7.29 (m, 1H), 7.27–7.17 (m, 2H), 6.62 (s, 1H), 3.38 (s, 3H), 3.17 (d, *J* = 14.8 Hz, 1H), 3.11 (d, *J* = 14.8 Hz, 1H), 2.13 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.9, 140.0, 139.4, 138.9, 136.6, 135.9, 133.8, 131.9, 131.0, 130.0, 128.7, 127.4, 127.2, 126.4, 124.5, 124.1, 123.2, 121.6, 121.3, 110.7, 102.9, 59.1, 45.4, 38.8, 23.0.

HRMS (ESI) calcd for $C_{25}H_{21}CI_2N_2O_3S^+$ $[M+H]^+$: 499.0644; Found: 499.0641.

5,7-dimethyl-7-((pyridin-3-ylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5q)



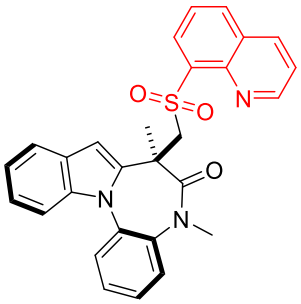
White solid, mp: 210-211 ºC. Yield: 86%.

^{1}H NMR (500 MHz, Chloroform-d) δ 8.76–8.68 (m, 1H), 8.63 (d, *J* = 2.3 Hz, 1H), 7. 80–7.73 (m, 1H), 7.67–7.61 (m, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.51–7.40 (m, 3H), 7.39–7.32 (m, 1H), 7.26–7.17 (m, 3H), 6.63 (s, 1H), 3.35 (s, 3H), 3.21 (d, *J* = 14.8 Hz, 1H), 3.16 (d, *J* = 14.9 Hz, 1H), 2.13 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.8, 154.1, 149.1, 140.0, 136.5, 136.2, 136.1, 135.9, 131.8, 128.6, 127.4, 126.5, 124.4, 124.1, 123.4, 123.1, 121.6, 121.3, 110.7, 102.9, 59.4, 45.4, 38.8, 22.9.

HRMS (ESI) calcd for $C_{24}H_{22}N_3O_3S^+$ $[M+H]^+$: 432.1376; Found: 432.1372.

5,7-dimethyl-7-((quinolin-8-ylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5r)



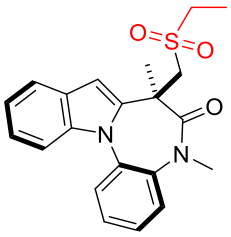
White solid, mp: 205-206 ºC. Yield: 84%.

^{1}H NMR (500 MHz, Chloroform-d) δ 8.87 (dd, *J* = 4.3, 1.8 Hz, 1H), 8.38 (dd, *J* = 7.3, 1.5 Hz, 1H), 8.21 (dd, *J* = 8.4, 1.8 Hz, 1H), 8.06 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.64–7.55 (m, 4H), 7.50–7.45 (m, 1H), 7.43–7.38 (m, 1H), 7.30–7.27 (m, 1H), 7.25–7.15 (m, 3H), 6.53 (s, 1H), 4.40–4.25 (m, 1H), 3.78–3.64 (m, 1H), 3.44 (s, 3H), 1.78 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.6, 151.4, 143.9, 141.3, 137.7, 136.9, 136.7, 136.0, 134.6, 131.9, 131.5, 128.9, 128.8, 127.2, 126.1, 125.7, 124.2, 124.2, 122.8, 122.2, 121.3, 121.1, 110.9, 102.2, 59.2, 45.6, 38.7, 22.8.

HRMS (ESI) calcd for $C_{28}H_{24}N_3O_3S^+$ $[M+H]^+$: 482.1533; Found: 482.1526.

7-((ethylsulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5s)



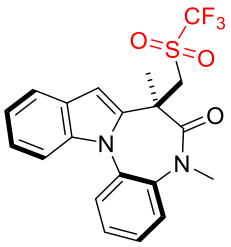
White solid, mp: 237-238 ºC. Yield: 81%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 (d, *J* = 8.1 Hz, 1H), 7.69–7.61 (m, 2H), 7.53–7.36 (m, 4H), 7.24–7.18 (m, 1H), 6.66 (s, 1H), 3.42 (s, 3H), 3.03 (d, *J* = 14.4 Hz, 1H), 2.93 (d, *J* = 14.4 Hz, 1H), 2.63–2.48 (m, 2H), 2.16 (s, 3H), 1.02 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.2, 169.1, 142.3, 140.8, 137.0, 136.9, 136.1, 135.9, 132.5, 132.1, 128.8, 128.8, 127.4, 126.6, 126.4, 124.6, 124.5, 124.4, 124.1, 123.0, 122.9, 121.5, 121.3, 121.1, 110.9, 110.9, 102.6, 100.2, 60.6, 54.3, 51.4, 49.7, 47.5, 44.8, 38.8, 38.7, 23.2, 19.6, 6.7, 6.5.

HRMS (ESI) calcd for $C_{21}H_{22}N_2O_3S^+$ $[M+H]^+$: 383.1424; Found: 383.1417.

5,7-dimethyl-7-(((trifluoromethyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino [1,7-*a*]indol-6(7*H*)-one (5t)



White solid, mp: 121-122 ºC. Yield: 83%.

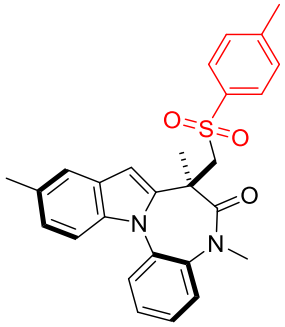
^{1}H NMR (500 MHz, Chloroform-d) δ 7.77 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.69–7.64 (m, 2H), 7.48–7.37 (m, 3H), 7.31–7.27 (m, 1H), 7.25–7.19 (m, 1H), 6.64 (s, 1H), 3.41 (s, 3H), 2.33–2.09 (m, 2H), 1.99 (s, 3H).

^{19}F NMR (471 MHz, Chloroform-d) δ -61.04.

^{13}C NMR (126 MHz, Chloroform-*d*) δ 170.1, 141.7, 136.9, 136.1, 132.2, 128.8, 127.5, 126.5, 124.7, 123.7, 122.8, 121.4, 121.2, 110.8, 102.1, 44.0, 38.7, 38.0 (d, *J* = 27.9 Hz), 23.0.

HRMS (ESI) calcd for $C_{20}H_{17}F_3N_2O_3S^+$ $[M+H]^+$: 423.0985; Found: 423.0981.

5,7,10-trimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5u)



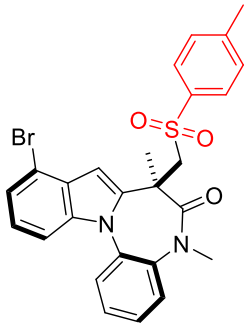
White solid, mp: 230-231 ºC. Yield: 67%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.51 (d, *J* = 7.9 Hz, 1H), 7.46–7.41 (m, 3H), 7.40–7.36 (m, 3H), 7.34–7.29 (m, 1H), 7.15 (d, *J* = 7.9 Hz, 2H), 7.04 (d, *J* = 6.6 Hz, 1H), 6.48 (s, 1H), 3.36 (s, 3H), 3.13 (d, *J* = 14.9 Hz, 1H), 3.03 (d, *J* = 14.7 Hz, 1H), 2.46–2.33 (m, 6H), 2.04 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.3, 144.9, 140.9, 137.2, 136.8, 134.4, 132.2, 130.8, 129.7, 129.1, 128.1, 127.0, 126.3, 124.5, 124.4, 124.3, 120.9, 110.5, 102.2, 59.2, 45.5, 38.8, 23.0, 21.7, 21.5.

HRMS (ESI) calcd for $C_{27}H_{27}N_2O_3S^+$ $[M+H]^+$: 459.1737; Found: 459.1736.

10-bromo-5,7-dimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5v)



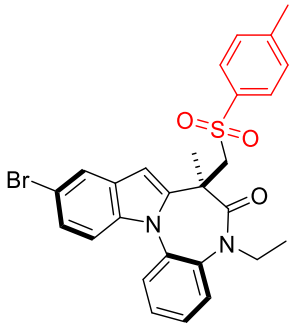
White solid, mp: 288-289 ºC. Yield: 57%.

^{1}H NMR (500 MHz, Chloroform-d) δ 7.73 (d, *J* = 2.0 Hz, 1H), 7.49–7.40 (m, 4H), 7.36 (d, *J* = 8.3 Hz, 3H), 7.29 (dd, *J* = 8.8, 1.9 Hz, 1H), 7.15 (d, *J* = 8.2 Hz, 2H), 6.50 (s, 1H), 3.37 (s, 3H), 3.09 (d, *J* = 14.7 Hz, 1H), 3.03 (d, *J* = 14.7 Hz, 1H), 2.35 (s, 3H), 2.02 (s, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 169.1, 145.0, 142.0, 137.2, 136.9, 134.8, 131.7, 130.5, 129.7, 128.1, 127.6, 126.4, 125.7, 124.5, 124.4, 123.7, 114.5, 112.3, 102.0, 58.9, 45.5, 38.8, 23.0, 21.7.

HRMS (ESI) calcd for $C_{26}H_{24}BrN_2O_3S^+$ $[M+H]^+$: 523.0686; Found: 523.0682.

10-bromo-5-ethyl-7-methyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5w)



White solid, mp: 206-207 ºC. Yield: 72% .

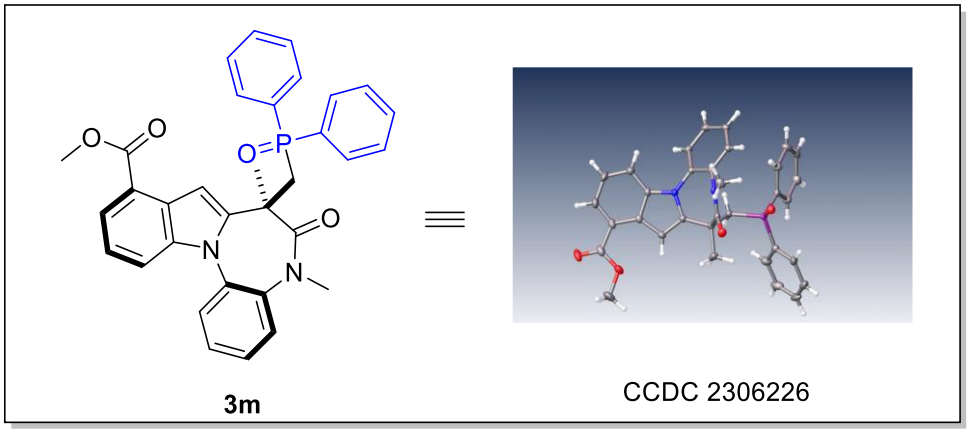
^{1}H NMR (500 MHz, Chloroform-d) δ 7.73 (d, *J* = 1.9 Hz, 1H), 7.54 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.48–7.40 (m, 3H), 7.37 – 7.33 (m, 3H), 7.28 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.13 (d, *J* = 7.9 Hz, 2H), 6.50 (s, 1H), 4.11–3.96 (m, 1H), 3.84–3.72 (m, 1H), 3.06 (s, 2H), 2.34 (s, 3H), 2.03 (s, 3H), 1.15 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, Chloroform-*d*) δ 168.1, 144.9, 142.2, 137.3, 136.1, 134.8, 132.5, 130.6, 129.7, 128.0, 127.7, 126.7, 125.7, 124.8, 124.7, 123.7, 114.5, 112.3, 102.1, 58.8, 46.7, 45.7, 23.0, 21.6, 13.4.

HRMS (ESI) calcd for $C_{27}H_{26}BrN_2O_3S^+$ $[M+H]^+$: 537.0842; Found: 537.0837.

5 X-ray crystallographic data

Crystal structure of compound 3m




```
Bond precision:   C-C = 0.0022 A          Wavelength=1.54178

Cell:             a=9.7645(2)     b=35.2767(6)        c=8.4612(1)
                  alpha=90        beta=108.393(1)     gamma=90
Temperature:      100 K

                  Calculated                  Reported
Volume            2765.65(8)                  2765.65(8)
Space group       P 21/c                      P 1 21/c 1
Hall group        -P 2ybc                     -P 2ybc
Moiety formula    C33 H29 N2 O4 P             C33 H29 N2 O4 P
Sum formula       C33 H29 N2 O4 P             C33 H29 N2 O4 P
Mr                548.55                      548.55
Dx,g cm-3         1.317                       1.317
Z                 4                           4
Mu (mm-1)         1.219                       1.219
F000              1152.0                      1152.0
F000'             1156.45
h,k,lmax          11,42,10                    11,42,10
Nref              5062                        5033
Tmin,Tmax         0.661,0.685                 0.634,0.753
Tmin'             0.599

Correction method= # Reported T Limits: Tmin=0.634 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 68.232

R(reflections)= 0.0380( 4836)                wR2(reflections)=
                                             0.0947( 5033)
S = 1.074                  Npar= 365
```

Bond precision: C-C = 0.0022 A Wavelength=1.54178

Cell: a=9.7645(2) b=35.2767(6) c=8.4612(11)

alpha=90 beta=108.393(1) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	2765.65(8)	2765.65(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C_{33} H_{29} N_2 O_4 P	C_{33} H_{29} N_2 O_4 P
Sum formula	C_{33} H_{29} N_2 O_4 P	C_{33} H_{29} N_2 O_4 P
Mr	548.55	548.55
Dx,g cm^{-3}	1.317	1.317
Z	4	4
Mu (mm^{-1})	1.219	1.219
F000	1152.0	1152.0
F000’	1156.45	
h,k,lmax	11,42,10	11,42,10
Nref	5062	5033
Tmin,Tmax	0.661,0.685	0.634,0.753
Tmin’		

Correction method= # Reported T Limits: Tmin=0.634 Tmax=0.753

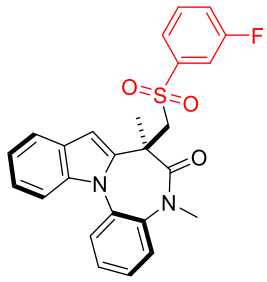
AbsCorr = MULTI-SCAN

Data completeness = 0.994 Theta(max)= 68.232

R(reflections)= 0.0380(4836) wR2(reflections)= 0.0947(5033)

S = 1.074 Npar= 365

Crystal structure of compound 5i



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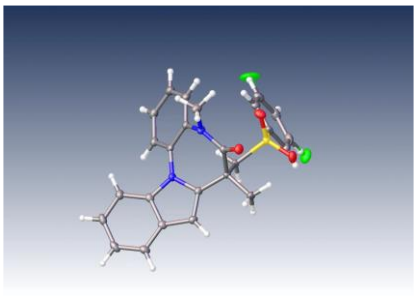


5i CCDC 2306225

```
Bond precision:   C-C = 0.0030 A          Wavelength=1.54178

Cell:              a=8.8308(3)      b=12.2131(4)      c=19.0148(6)
                   alpha=90         beta=90           gamma=90
Temperature:       100 K

                  Calculated                  Reported
Volume            2050.77(12)                 2050.77(12)
Space group       P n a 21                    P n a 21
Hall group        P 2c -2n                    P 2c -2n
Moiety formula    C25 H21 F N2 O3 S           C25 H21 F N2 O3 S
Sum formula       C25 H21 F N2 O3 S           C25 H21 F N2 O3 S
Mr                448.50                      448.50
Dx,g cm-3         1.453                       1.453
Z                 4                           4
Mu (mm-1)         1.753                       1.753
F000              936.0                       936.0
F000'             940.14
h,k,lmax          10,14,22                    10,14,22
Nref              3761[ 1942]                 3698
Tmin,Tmax         0.512,0.541                 0.610,0.753
Tmin'             0.464

Correction method= # Reported T Limits: Tmin=0.610 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.90/0.98        Theta(max)= 68.301

R(reflections)= 0.0218( 3681)                wR2(reflections)=
                                             0.0576( 3698)
S = 1.068                  Npar= 301
```

Bond precision: C-C = 0.0030 A Wavelength=1.54178

Cell: a=8.8308(3) b=12.2131(4) c=19.0148(6)

alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2050.77 (12)	2050.77 (12)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C_{25} H_{21} F N_2 O_3 S	C_{25} H_{21} F N_2 O_3 S
Sum formula	C_{25} H_{21} F N_2 O_3 S	C_{25} H_{21} F N_2 O_3 S
Mr	448.50	448.50
Dx,g cm^{-3}	1.453	1.453
Z	4	4
Mu (mm^{-1})	1.753	1.753
F000	936.0	936.0
F000’	940.14	
h,k,lmax	10,14,22	10,14,22
Nref	3761[1942]	3698
Tmin,Tmax	0.512,0.541	0.610,0.753
Tmin’	0.464	

Correction method= # Reported T Limits: Tmin=0.610 Tmax=0.753

AbsCorr = MULTI-SCAN

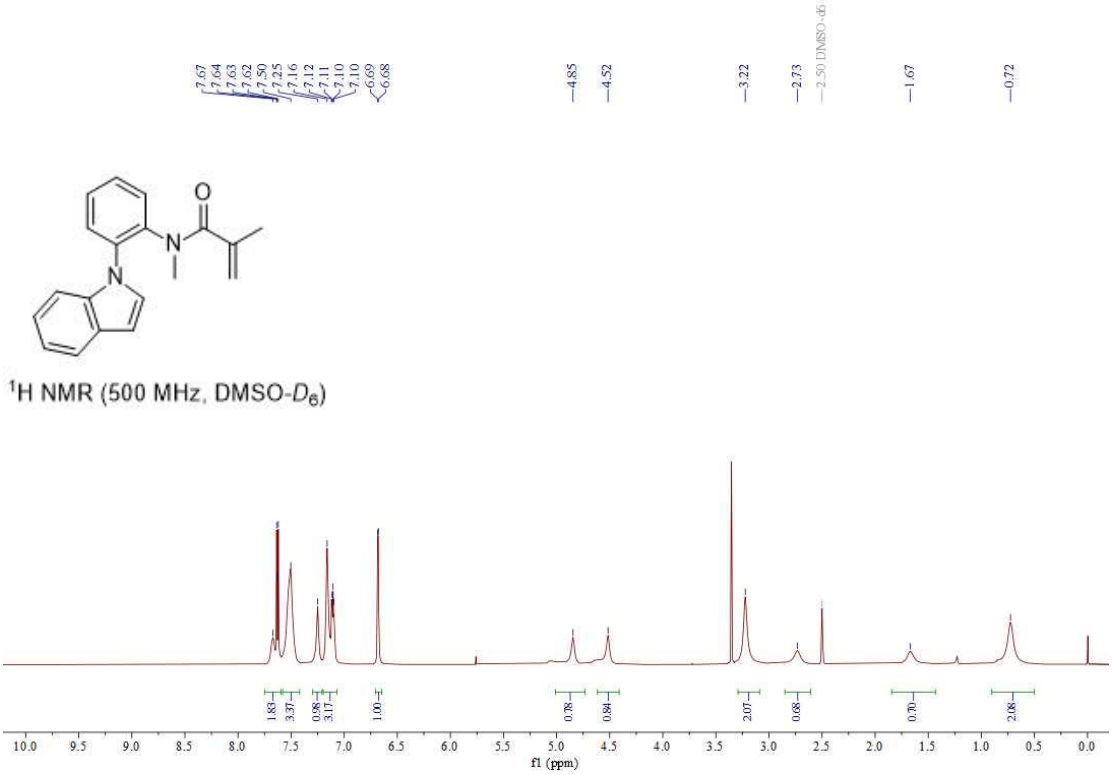
Data completeness = 1.90/0.98 Theta(max)= 68.301

R(reflections)= 0.0218(1689) wR2(reflections)= 0.0576(3698)

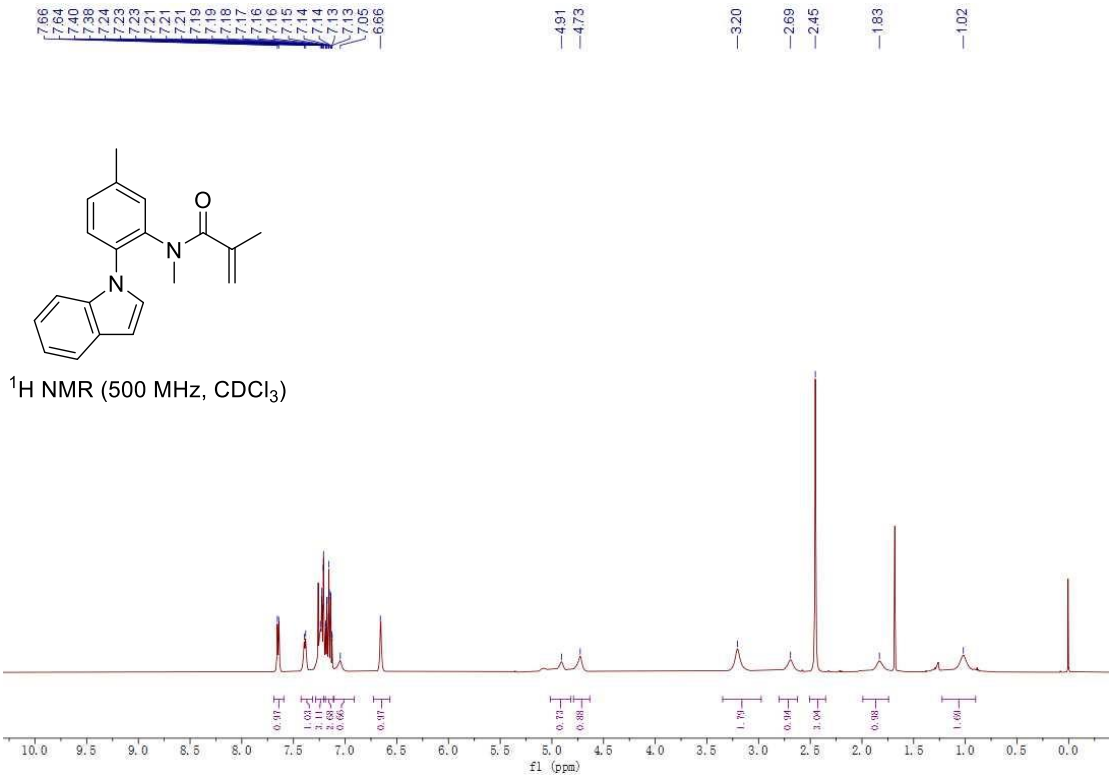
S = 1.074 Npar= 365

6 NMR spectra

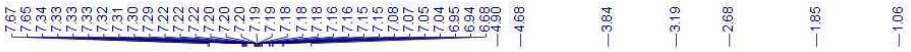
***N*-(2-(1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1a)**

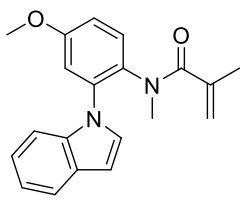


***N*-(2-(1*H*-indol-1-yl)-5-methylphenyl)-*N*-methylmethacrylamide (1b)**

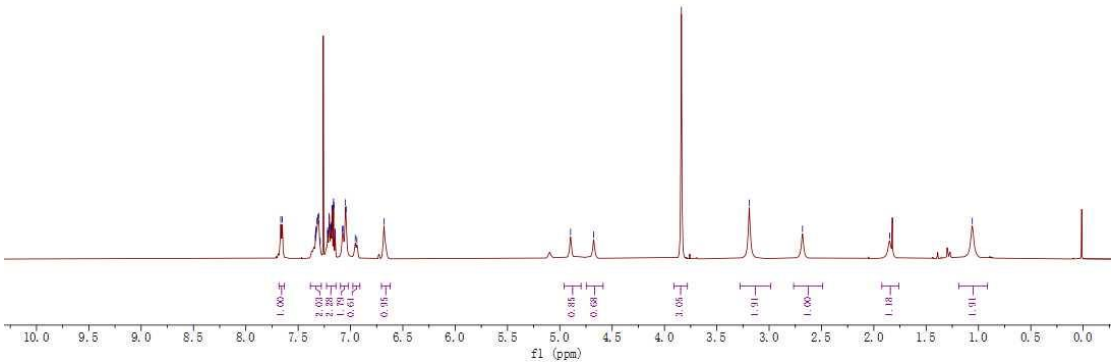


***N*-(2-(1*H*-indol-1-yl)-4-methoxyphenyl)-*N*-methylmethacrylamide (1c)**

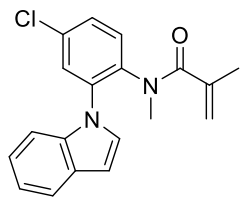




^{1}H NMR (500 MHz, $CDCl_3$)

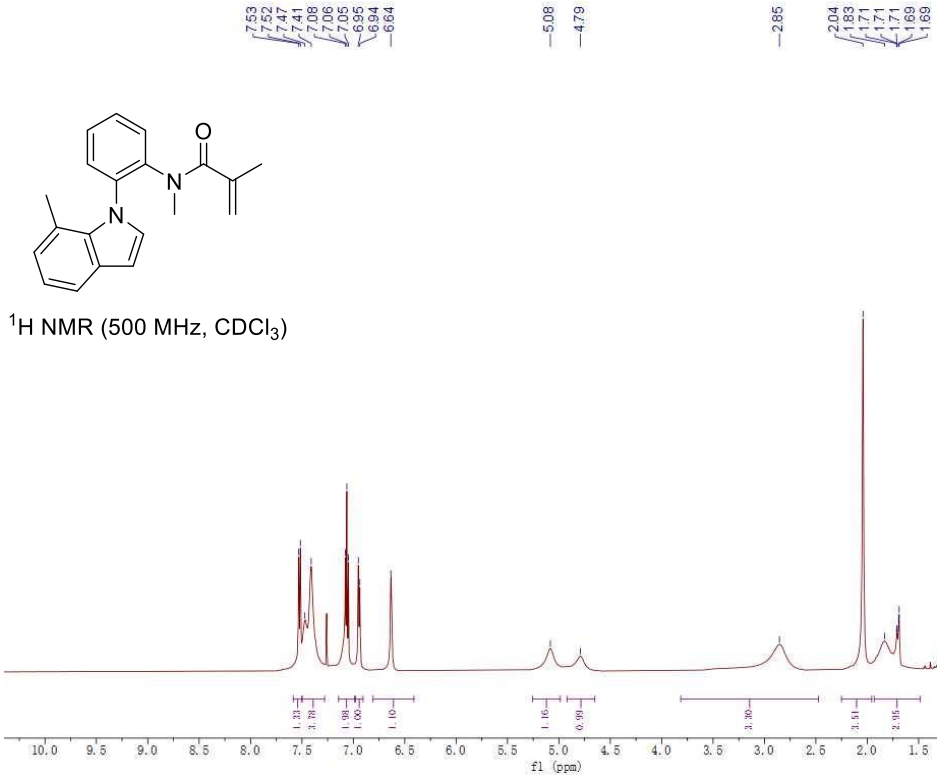


***N*-(4-chloro-2-(1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1d)**

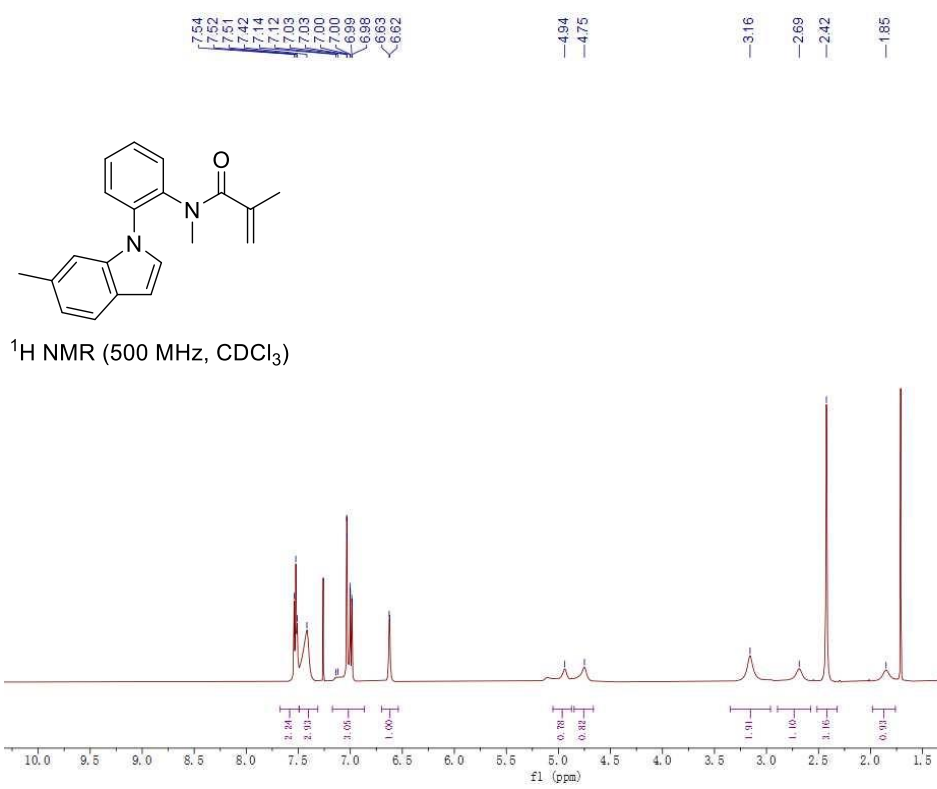


^{1}H NMR (500 MHz, $CDCl_3$)

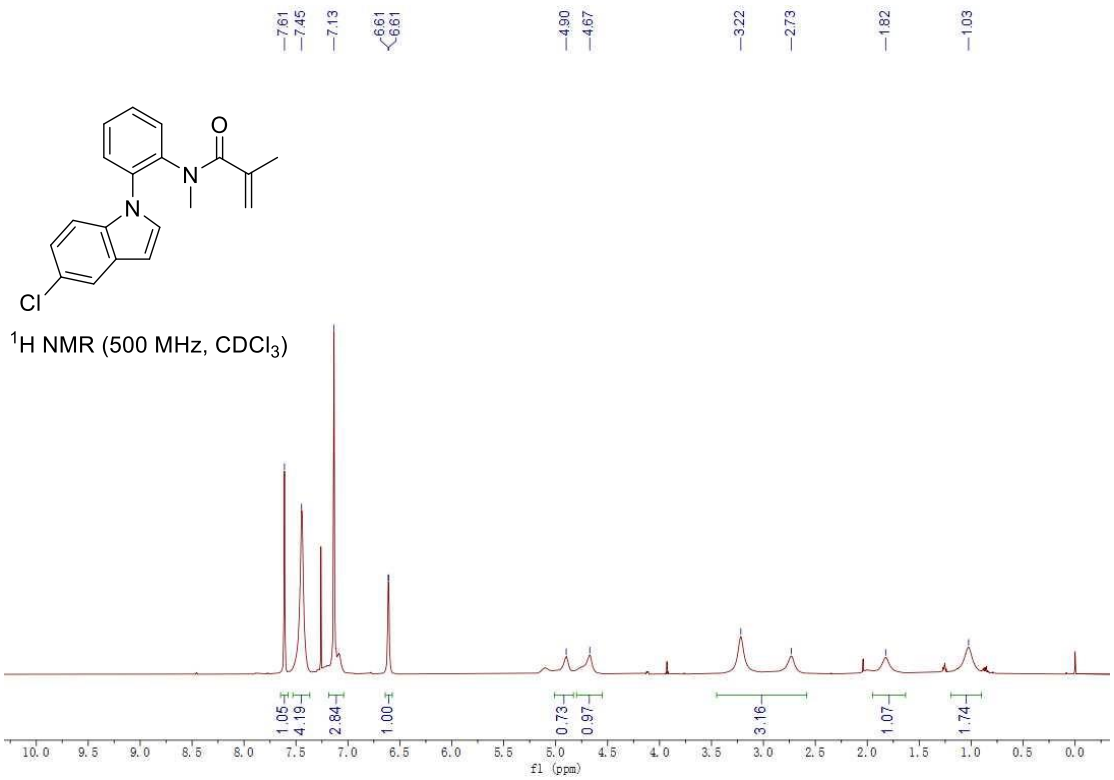
***N*-methyl-*N*-(2-(7-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1e)**



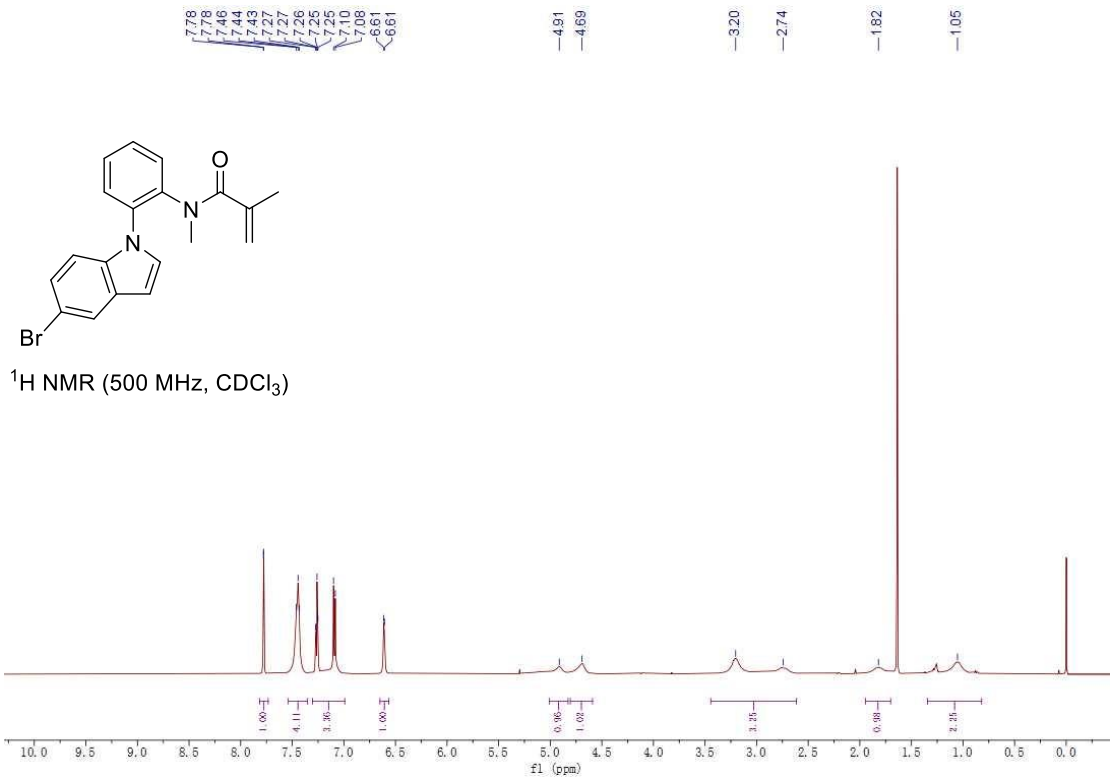
***N*-methyl-*N*-(2-(6-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1f)**



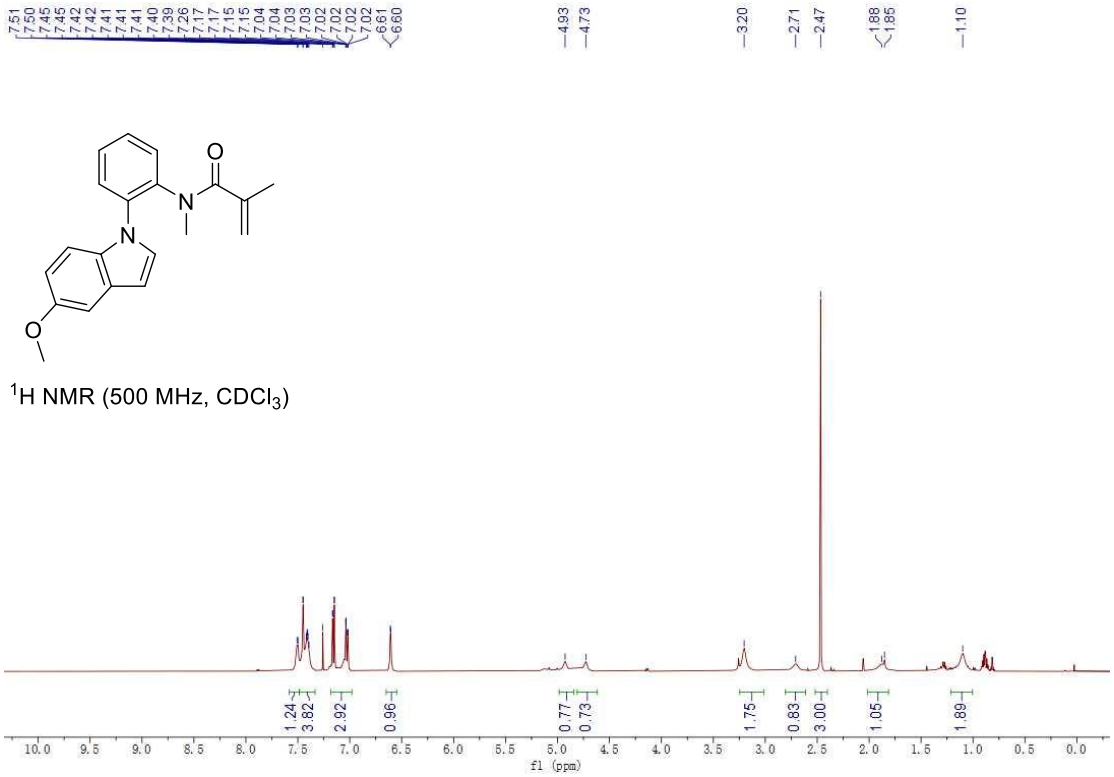
***N*-(2-(5-chloro-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1g)**



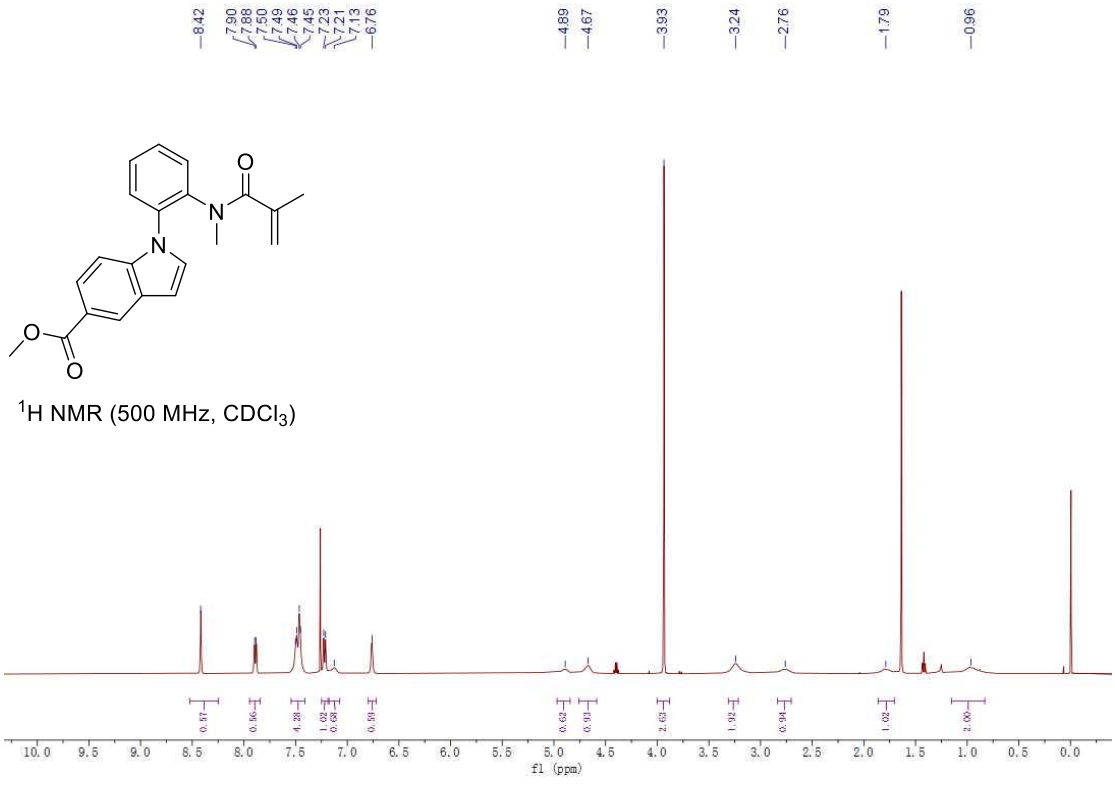
***N*-(2-(5-bromo-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1h)**



***N*-(2-(5-methoxy-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1i)**

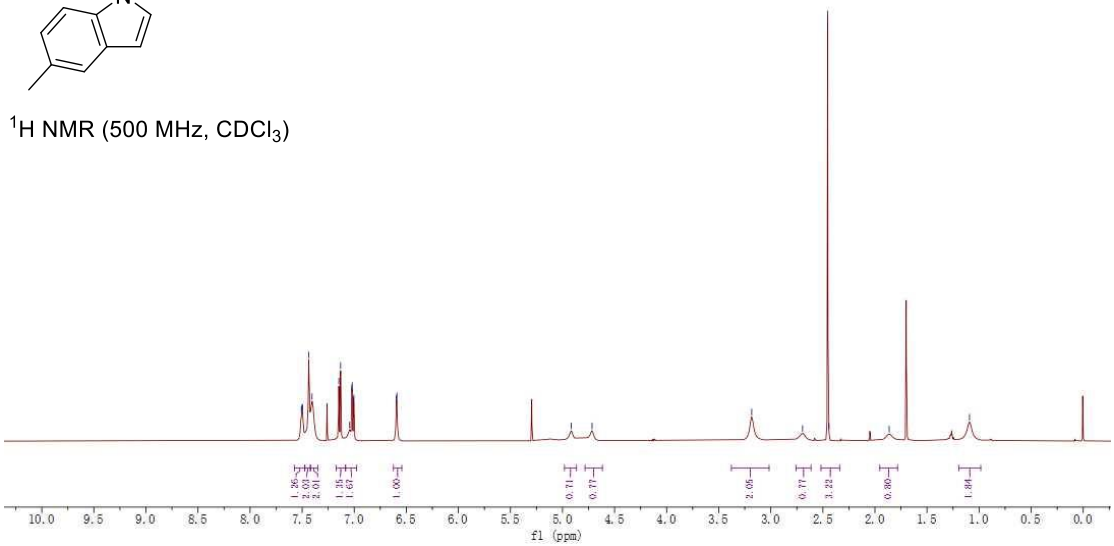


methyl 1-(2-(*N*-methylmethacrylamido)phenyl)-1*H*-indole-5-carboxylate (1j)



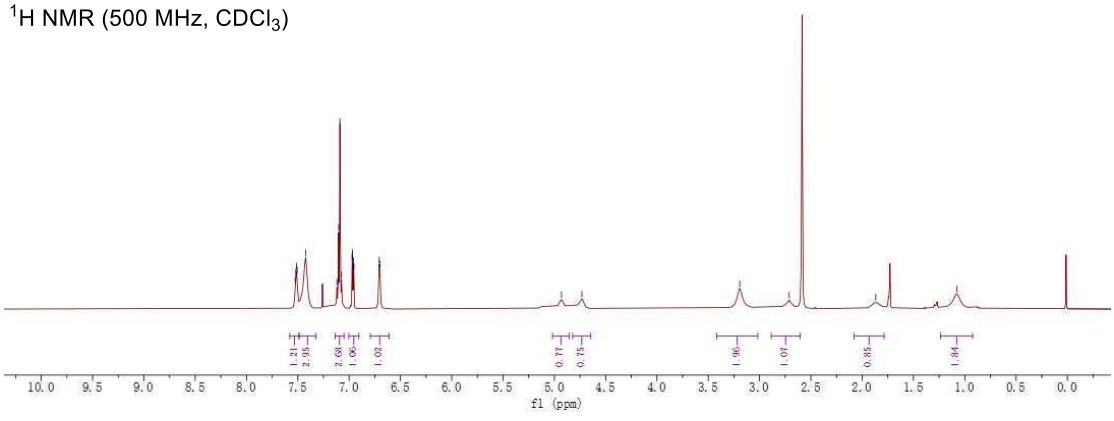
***N*-methyl-*N*-(2-(5-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1k)**

^{1}H NMR (500 MHz, $CDCl_3$)

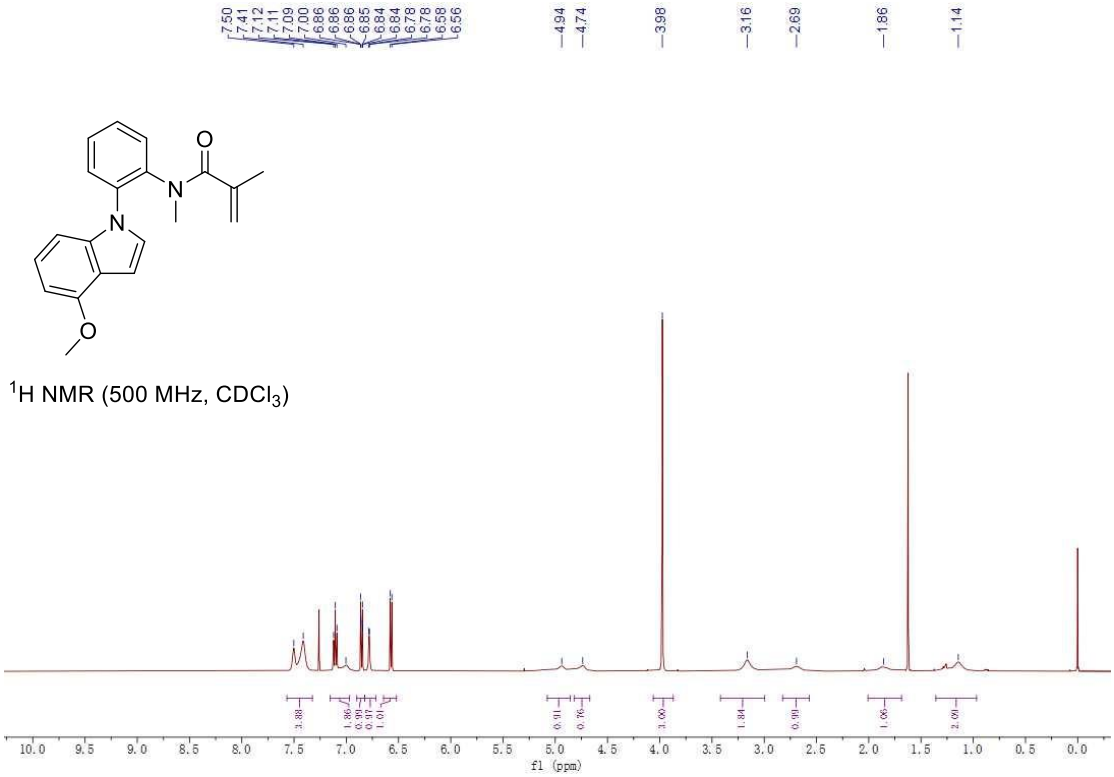


***N*-(2-(4-bromo-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1l)**

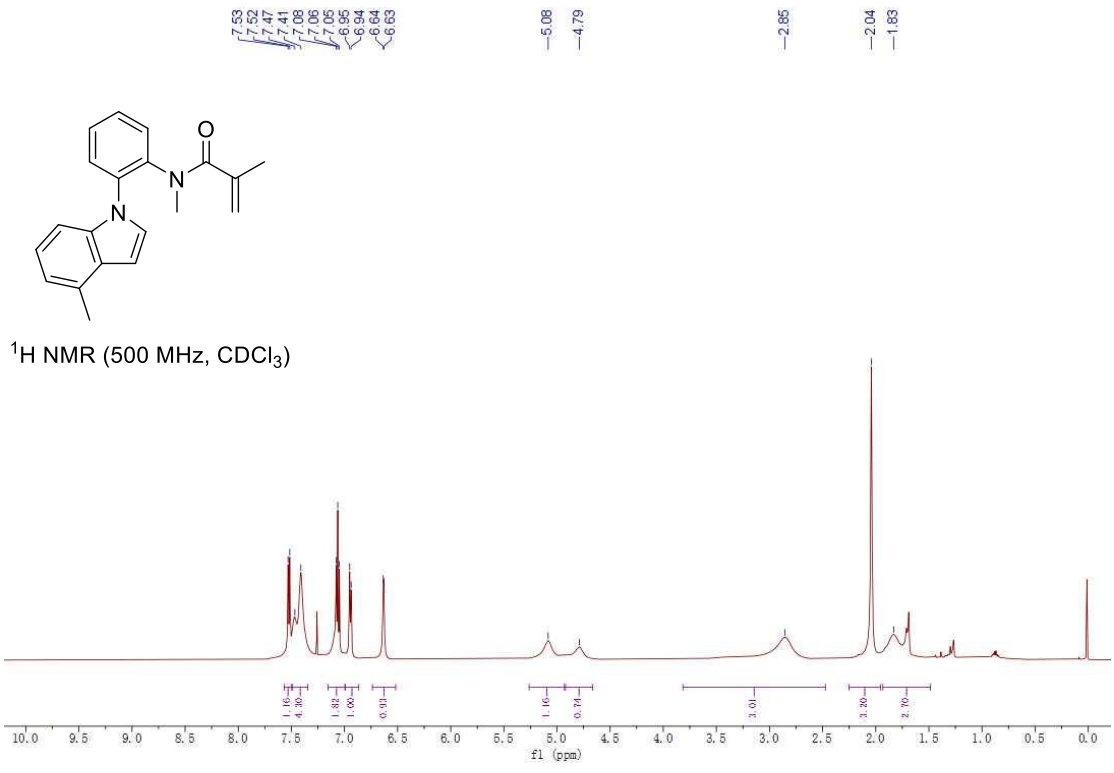
^{1}H NMR (500 MHz, $CDCl_3$)



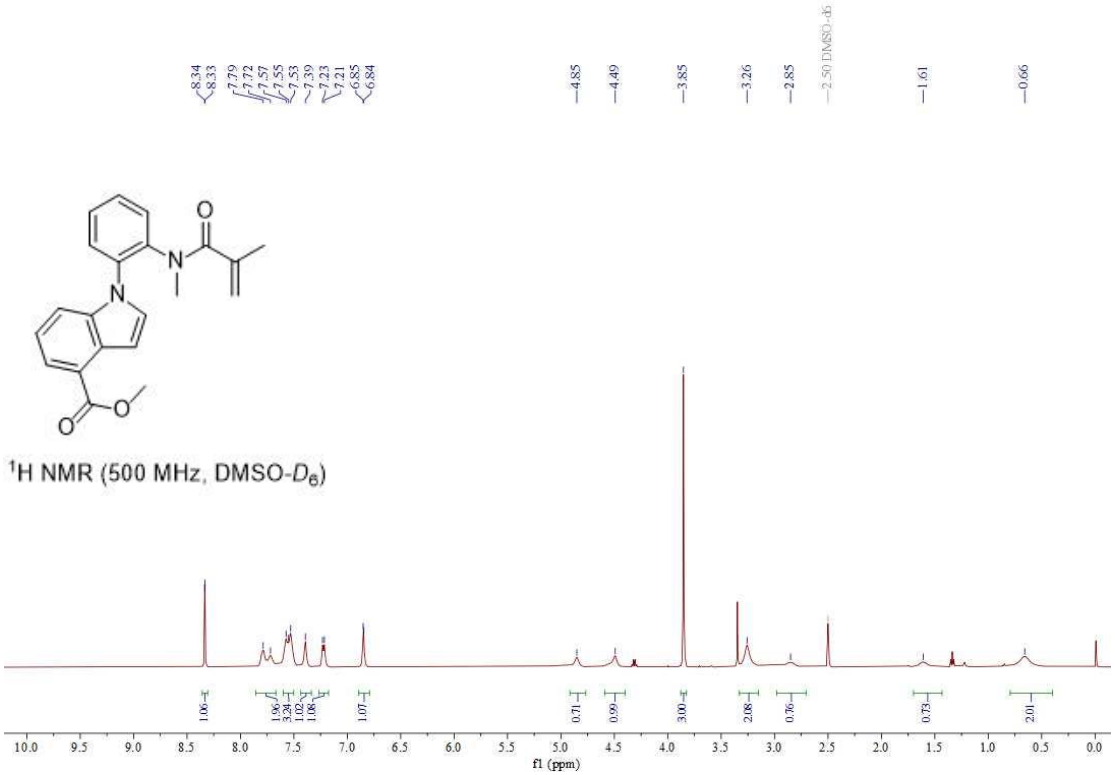
***N*-(2-(4-methoxy-1*H*-indol-1-yl)phenyl)-*N*-methylmethacrylamide (1m)**



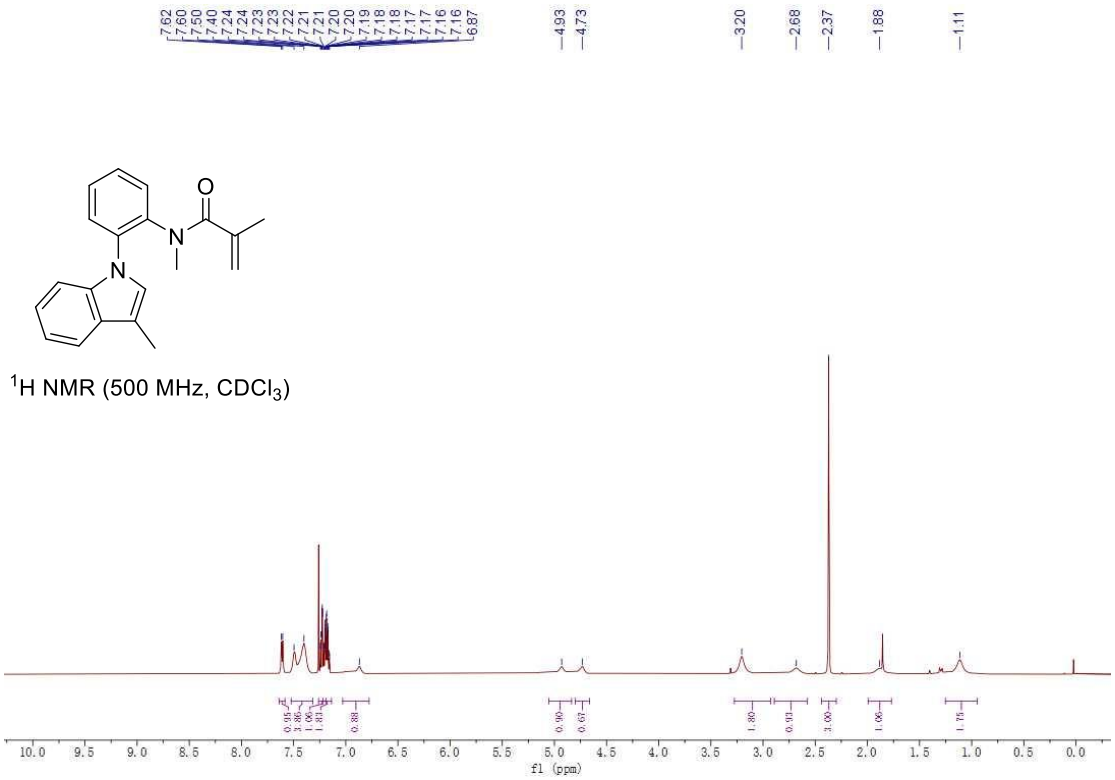
***N*-methyl-*N*-(2-(4-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1n)**



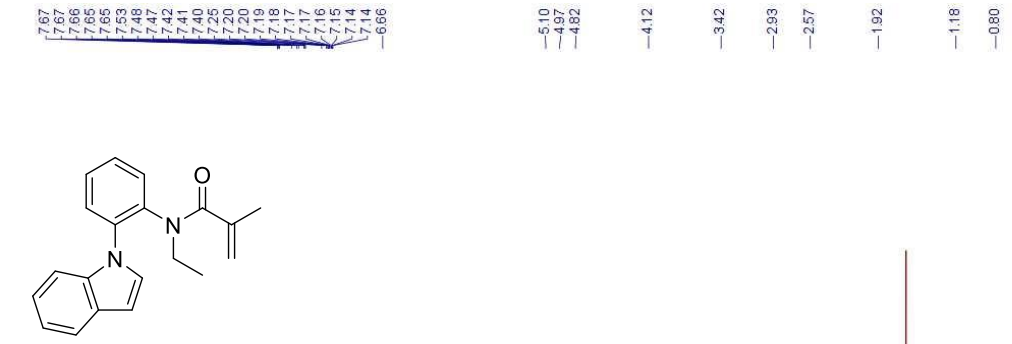
methyl 1-(2-(*N*-methylmethacrylamido)phenyl)-1*H*-indole-4-carboxylate (1o)



***N*-methyl-*N*-(2-(3-methyl-1*H*-indol-1-yl)phenyl)methacrylamide (1p)**

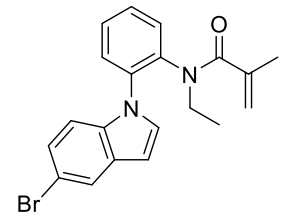


***N*-(2-(1*H*-indol-1-yl)phenyl)-*N*-ethylmethacrylamide (1q)**

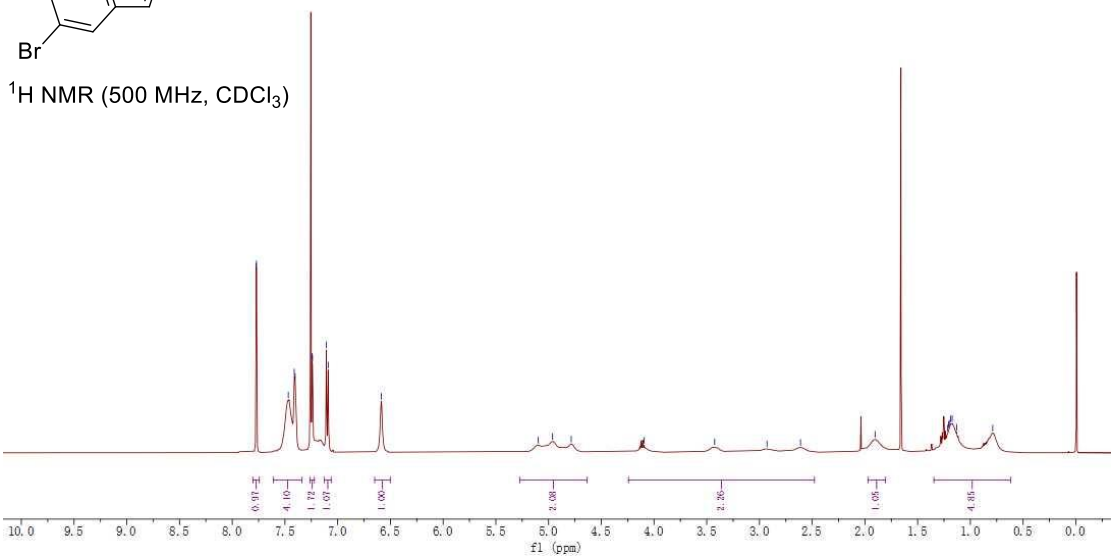


^{1}H NMR (500 MHz, $CDCl_3$)

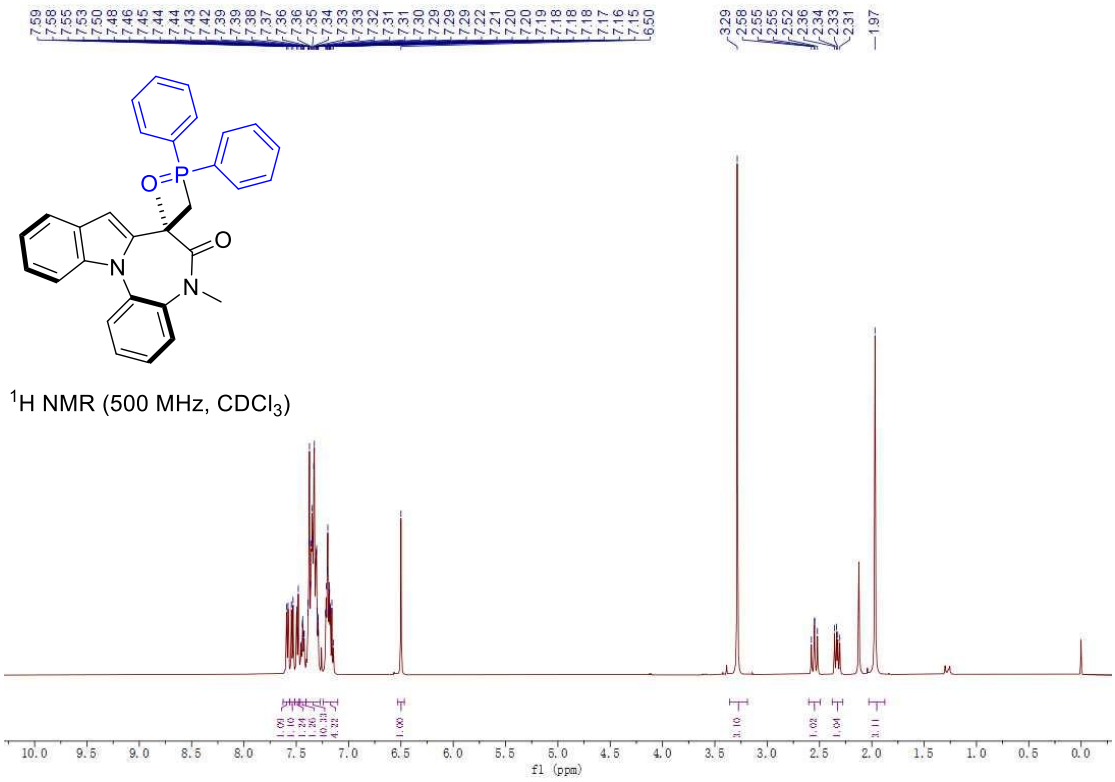
***N*-(2-(5-bromo-1*H*-indol-1-yl)phenyl)-*N*-ethylmethacrylamide (1r)**



^{1}H NMR (500 MHz, $CDCl_3$)

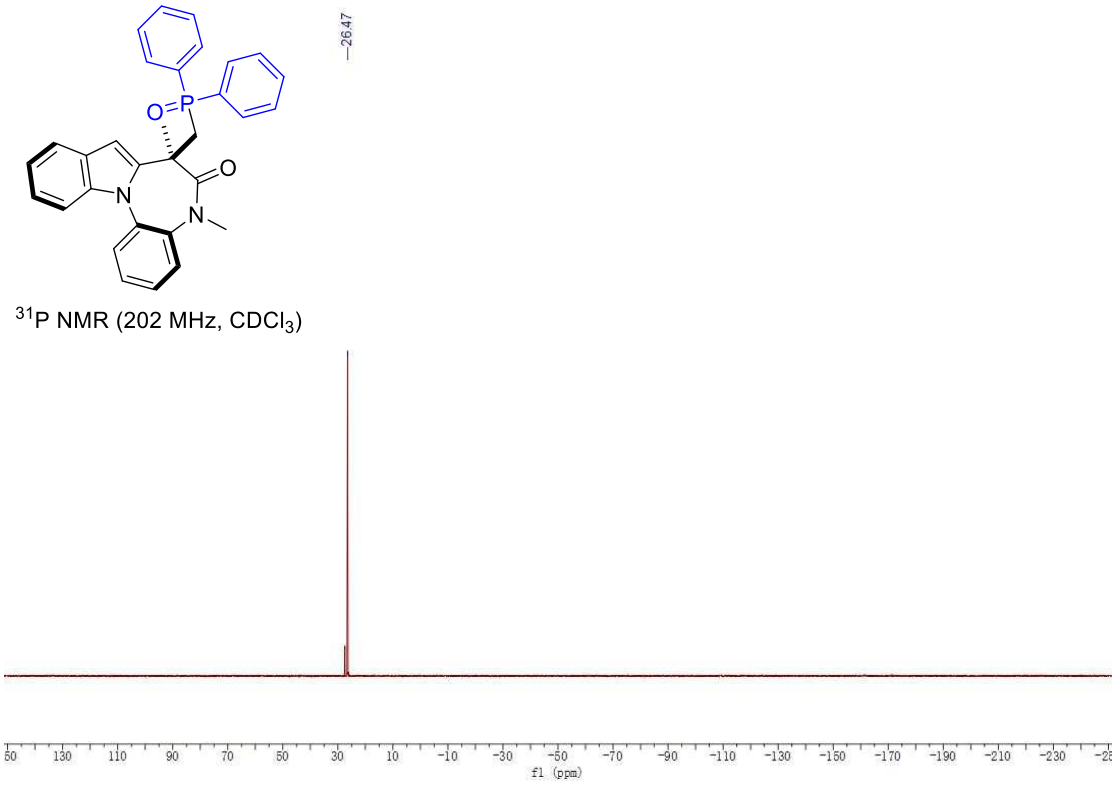


7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3a)



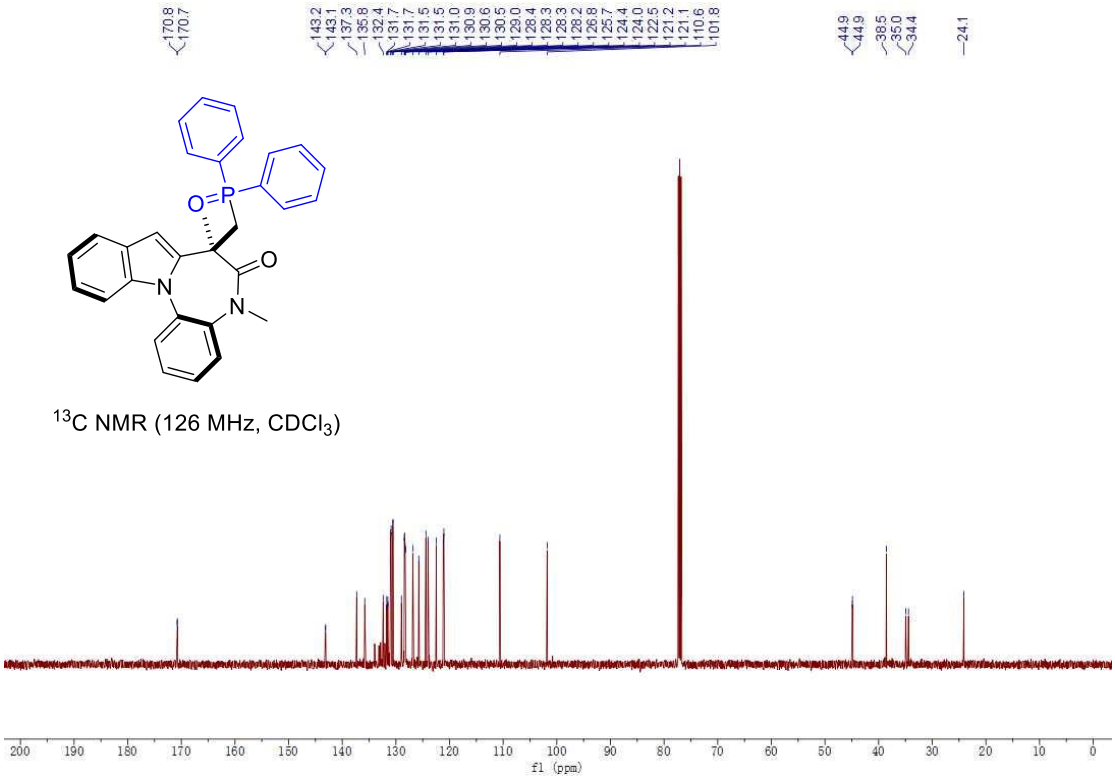
^{1}H NMR (500 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3a)

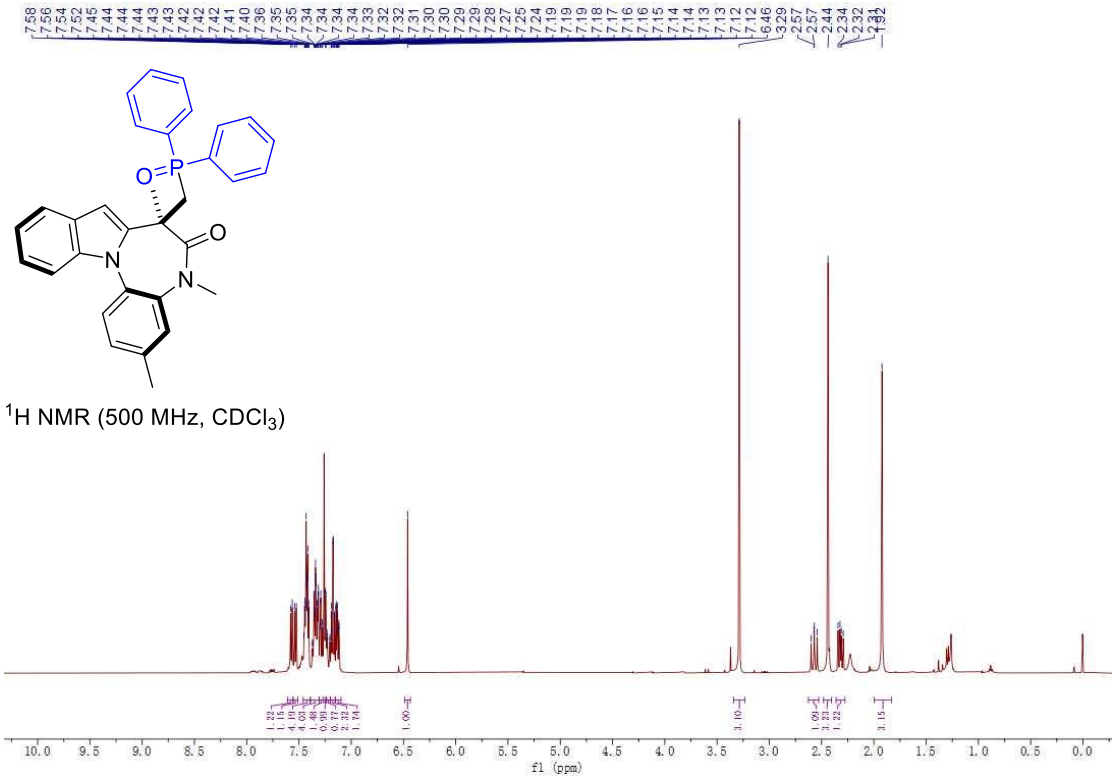


^{31}P NMR (202 MHz, $CDCl_3$)

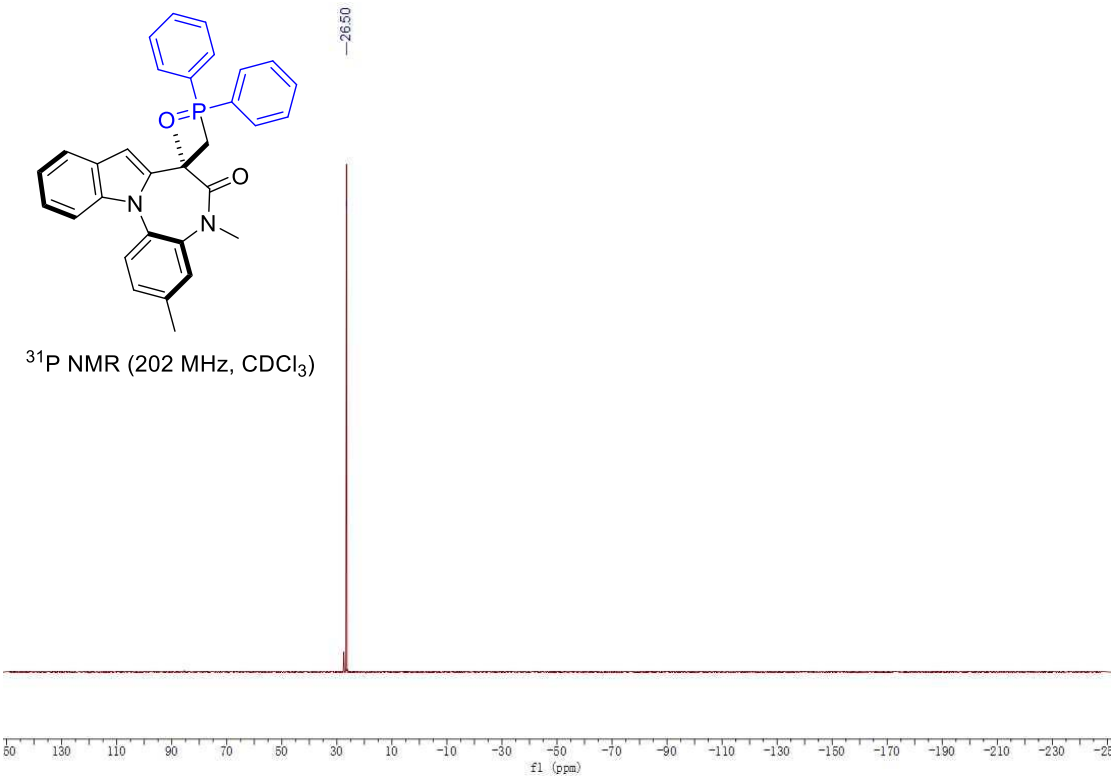
7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3a)



7-((diphenylphosphoryl)methyl)-3,5,7-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3b)

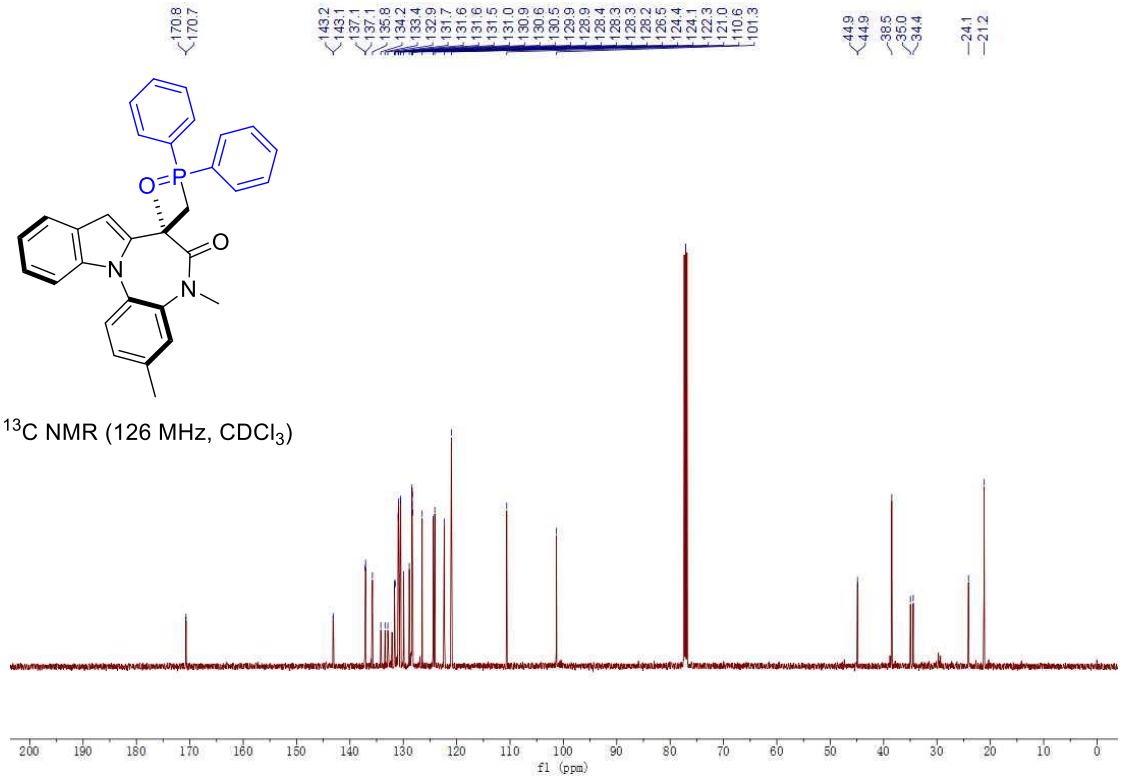


7-((diphenylphosphoryl)methyl)-3,5,7-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3b)



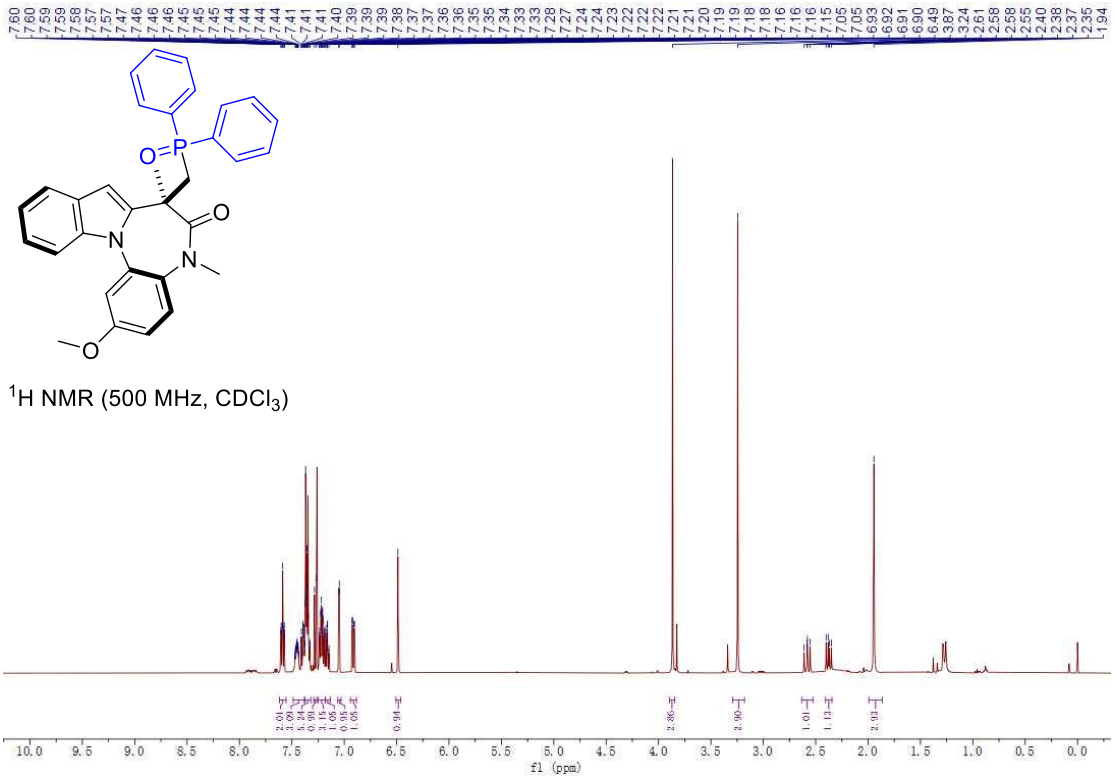
^{31}P NMR (202 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-3,5,7-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3b)



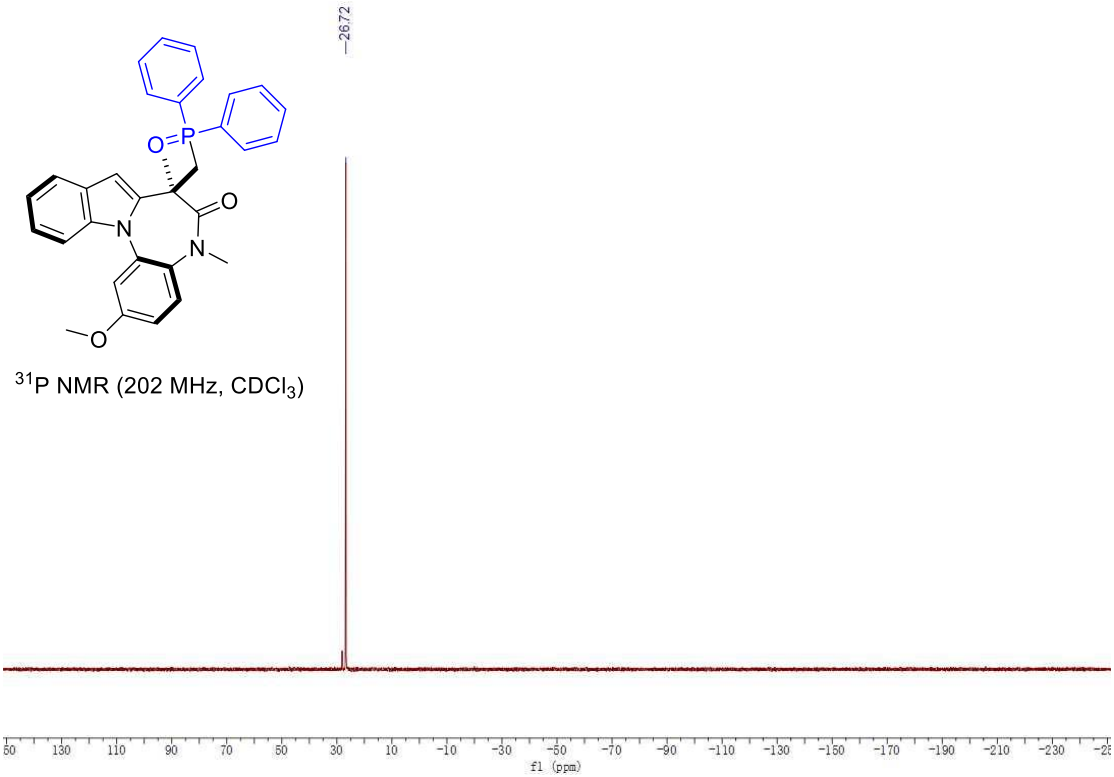
^{13}C NMR (126 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-3-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3c)



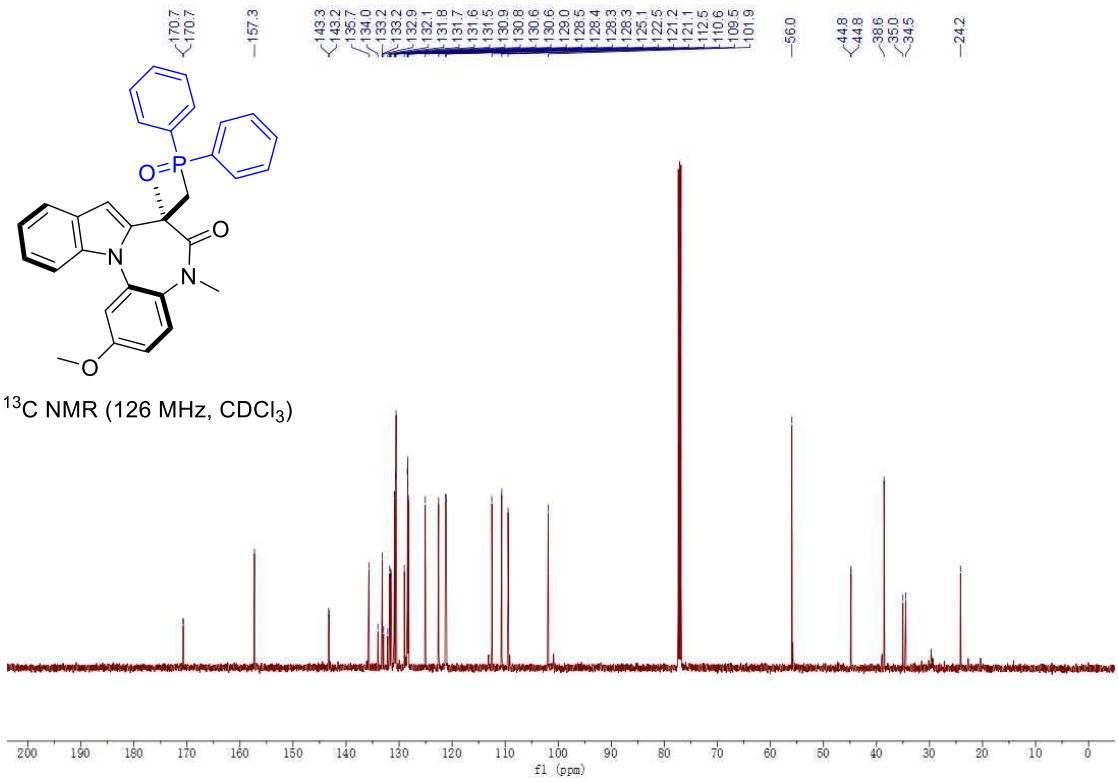
^{1}H NMR (500 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-3-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3c)

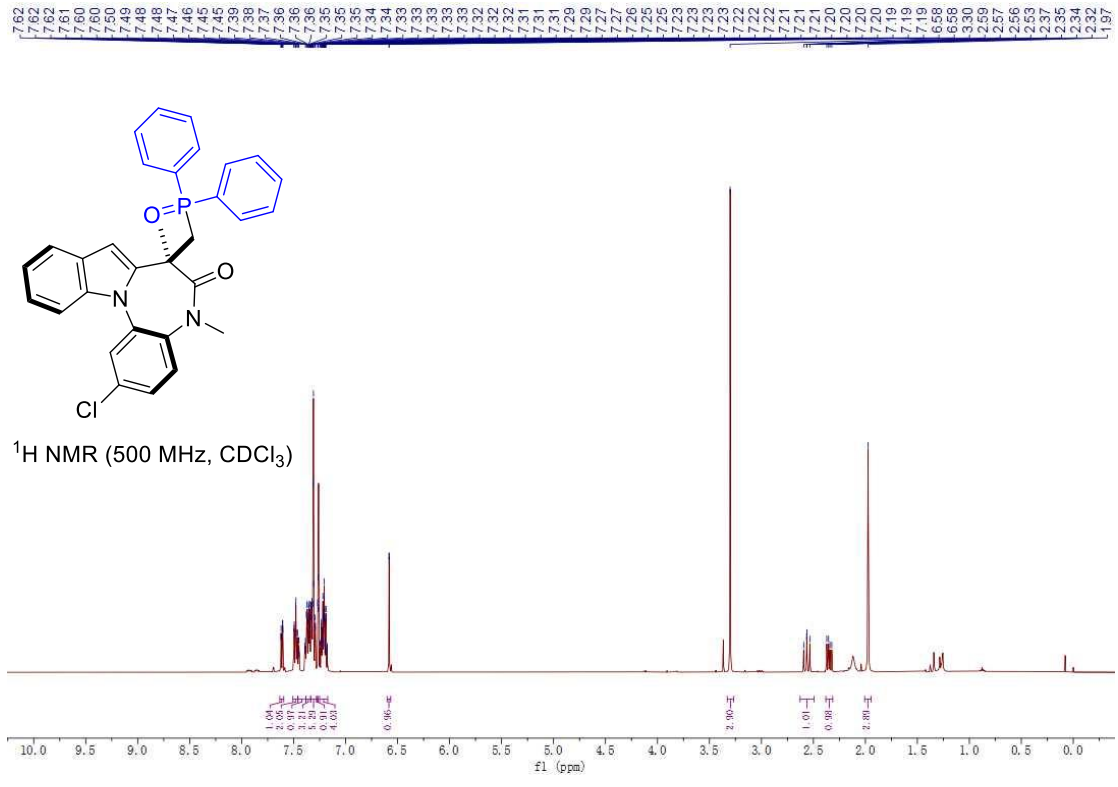


^{31}P NMR (202 MHz, $CDCl_3$)

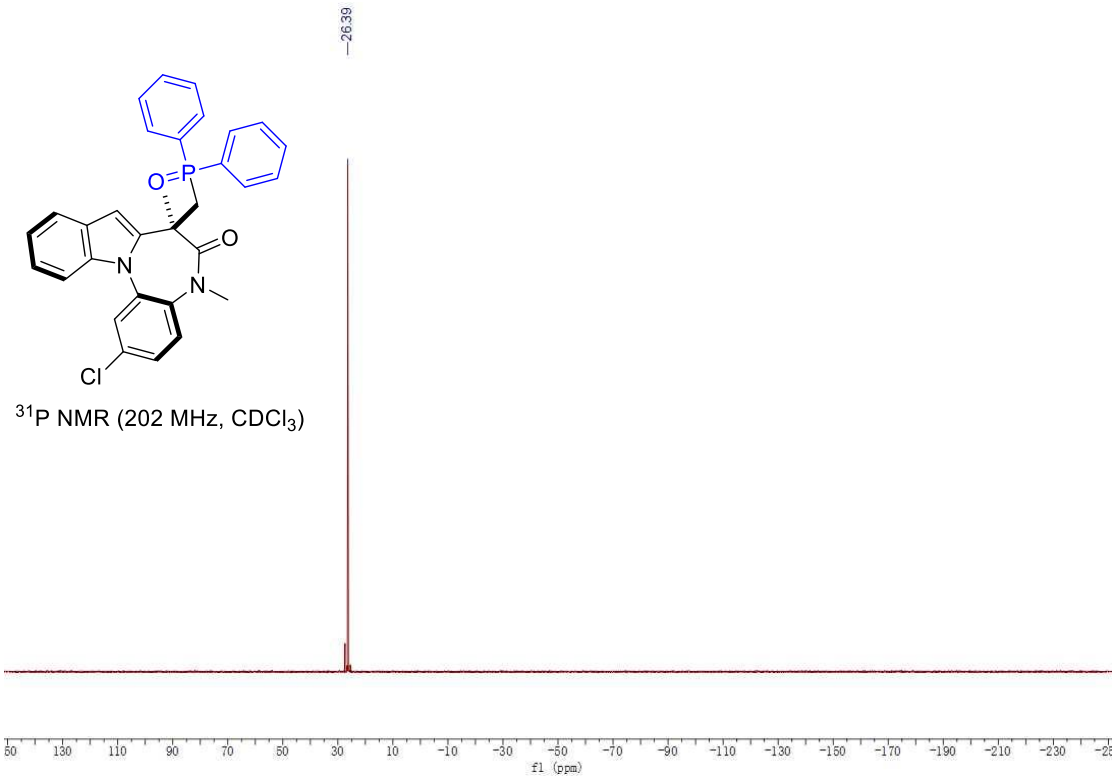
7-((diphenylphosphoryl)methyl)-3-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3c)



3-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3d)

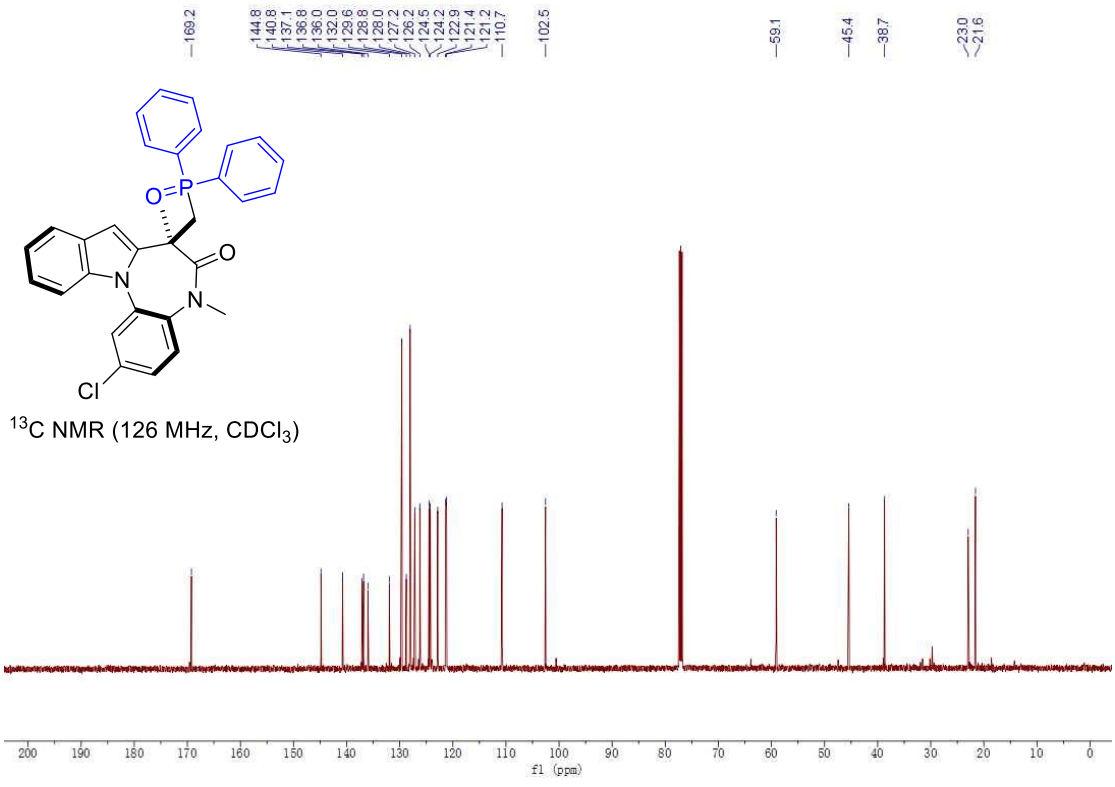


3-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3d)



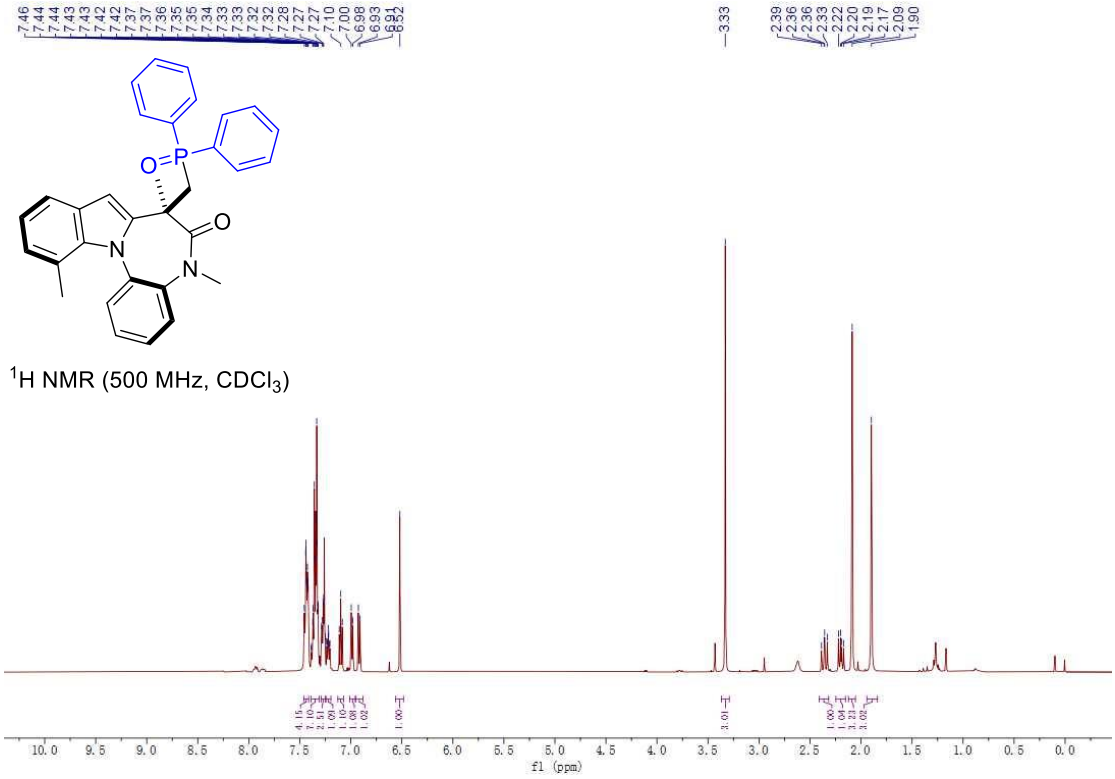
^{31}P NMR (202 MHz, $CDCl_3$)

3-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3d)

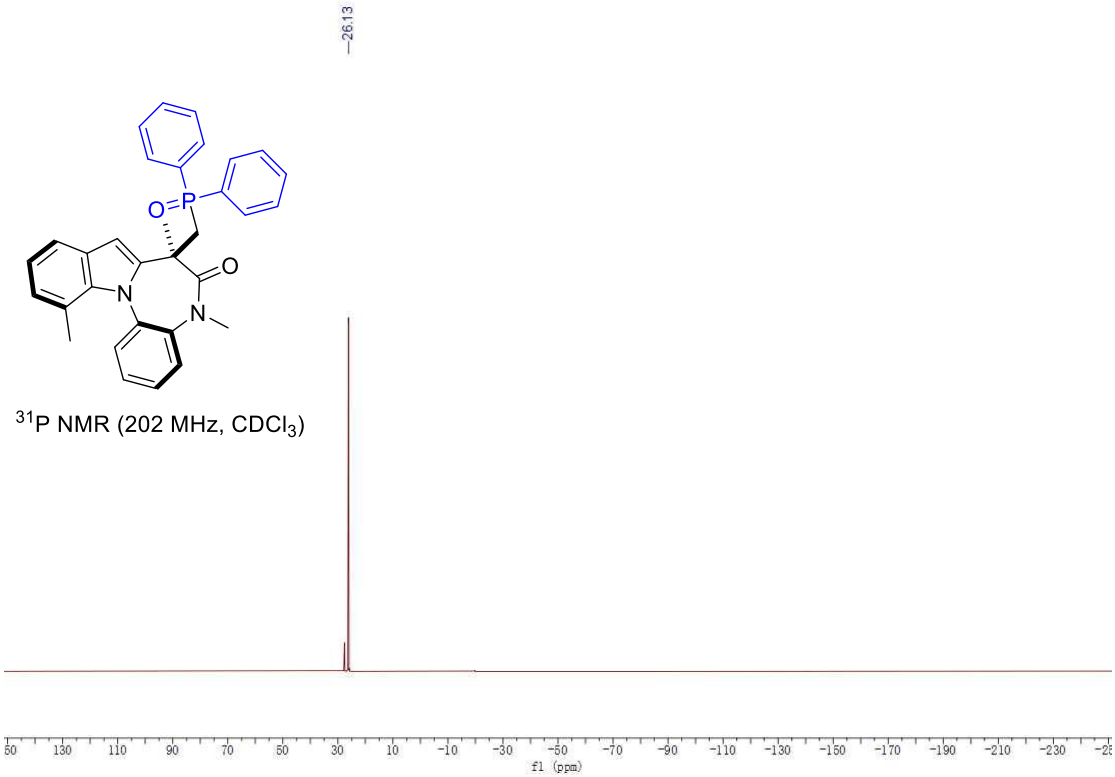


^{13}C NMR (126 MHz, $CDCl_3$)

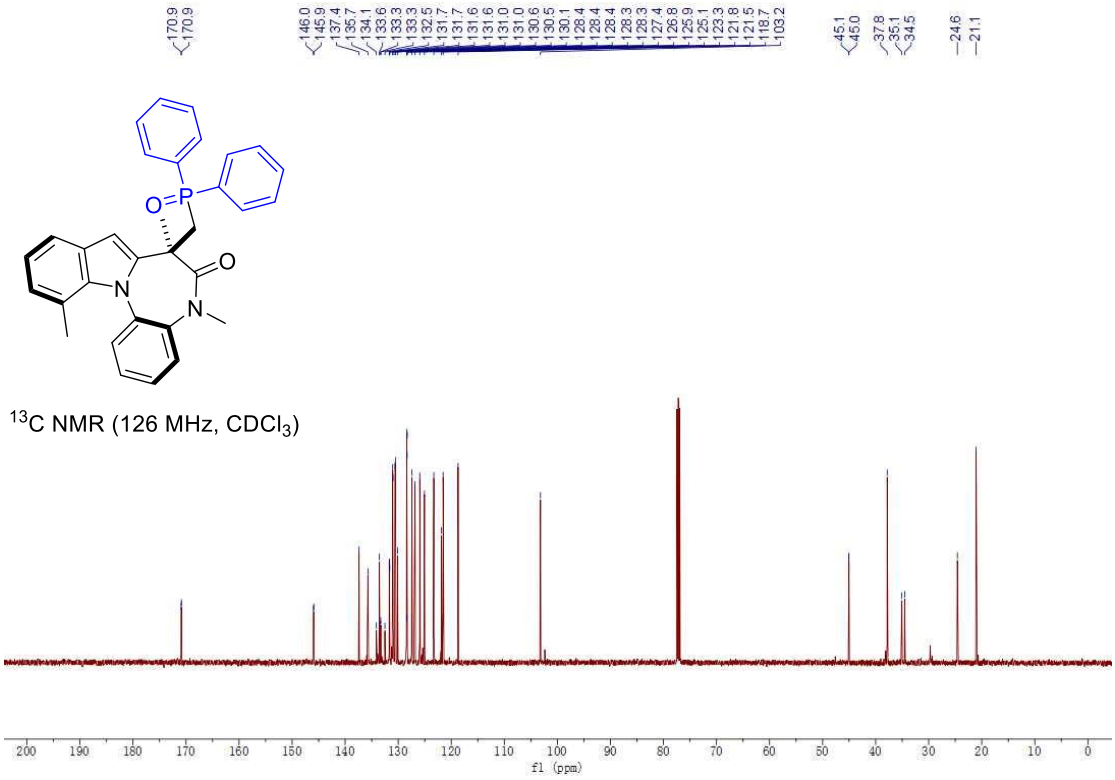
7-((diphenylphosphoryl)methyl)-5,7,12-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3e)



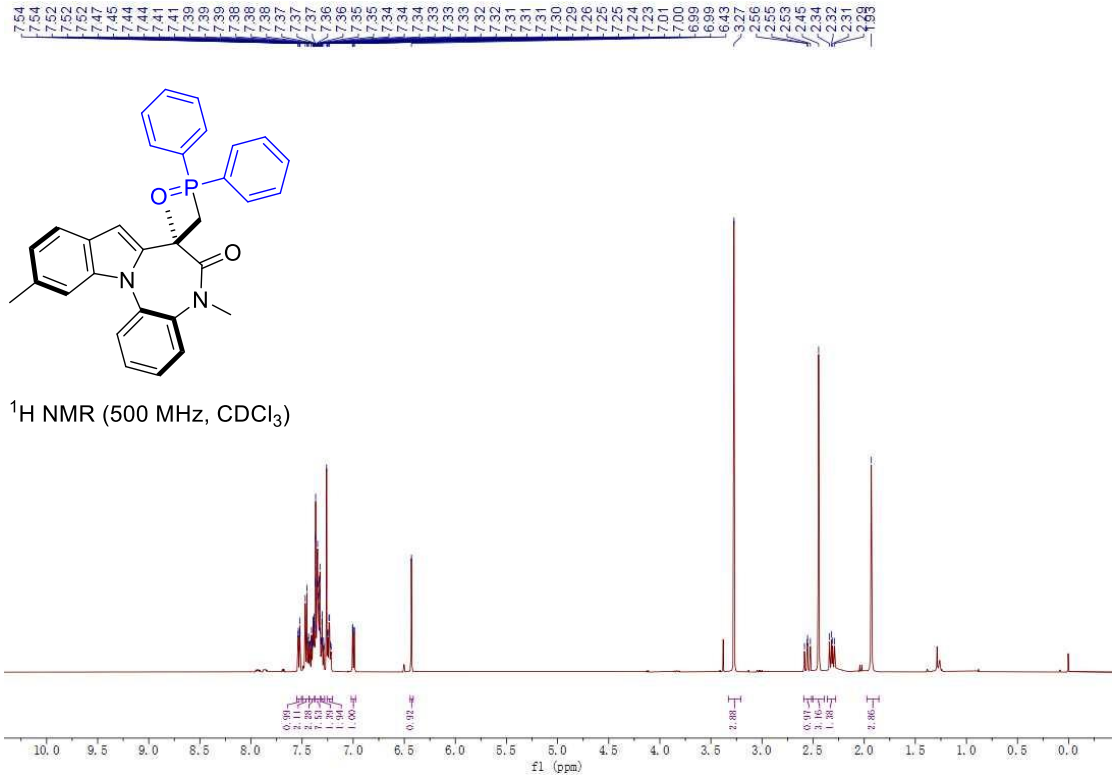
7-((diphenylphosphoryl)methyl)-5,7,12-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3e)



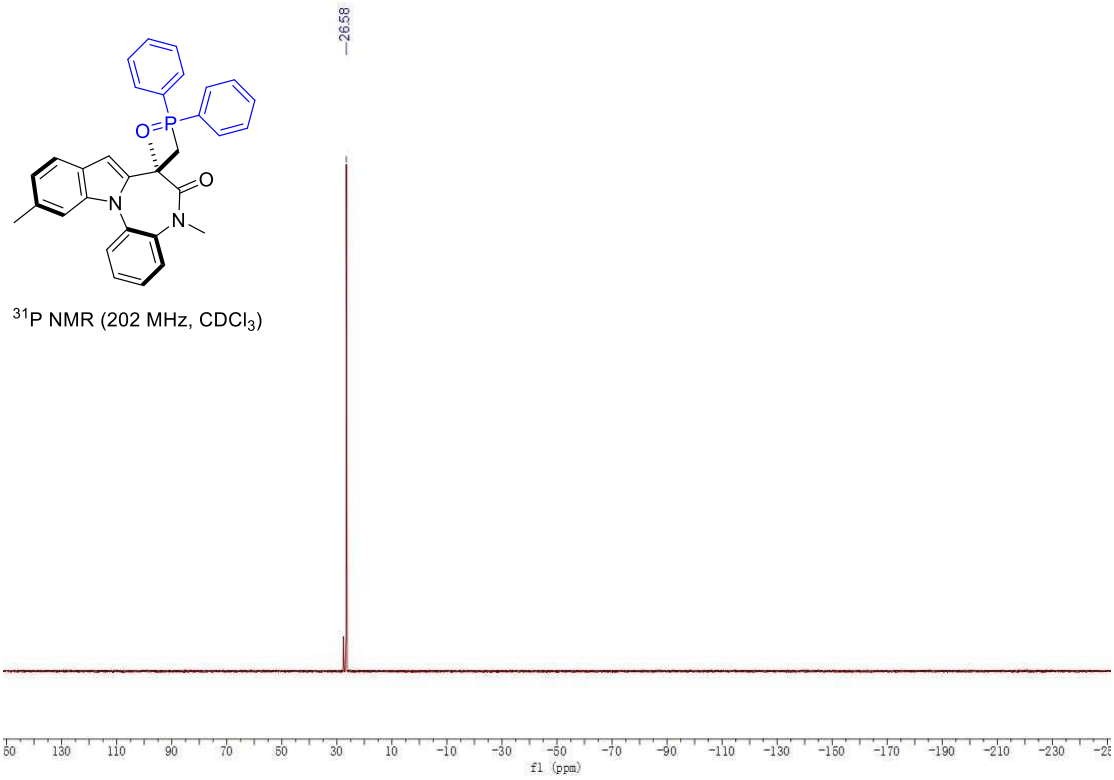
7-((diphenylphosphoryl)methyl)-5,7,12-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3e)



7-((diphenylphosphoryl)methyl)-5,7,11-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3f)

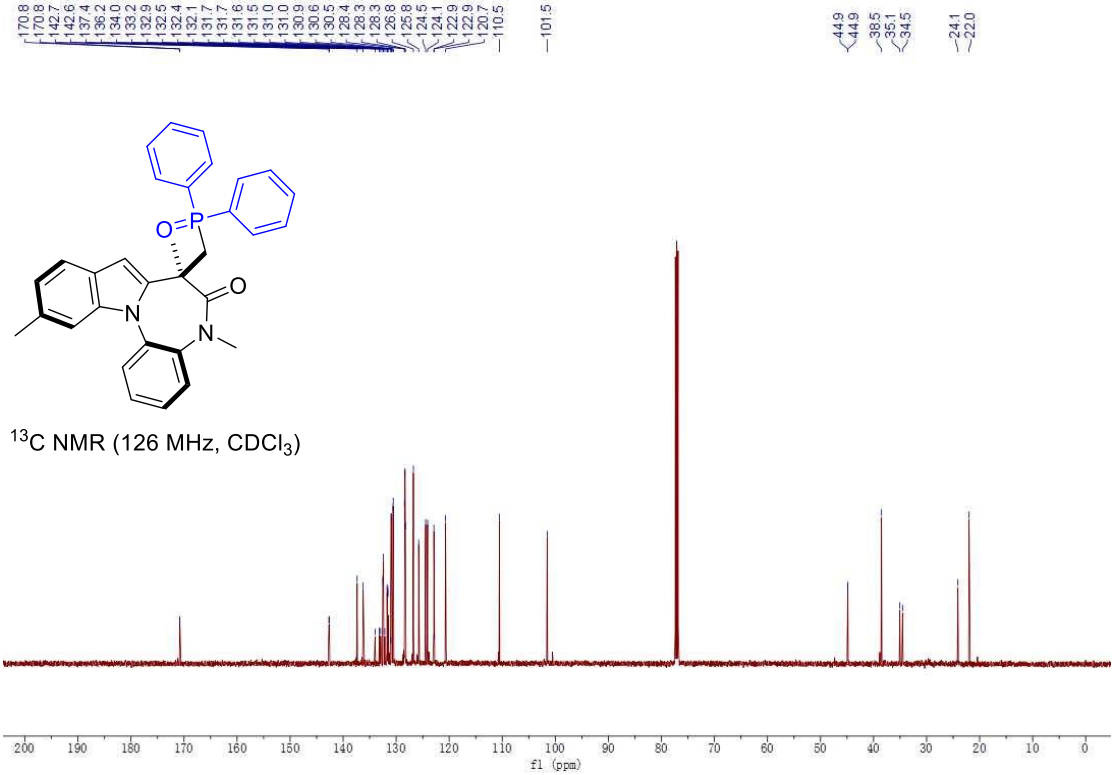


7-((diphenylphosphoryl)methyl)-5,7,11-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3f)



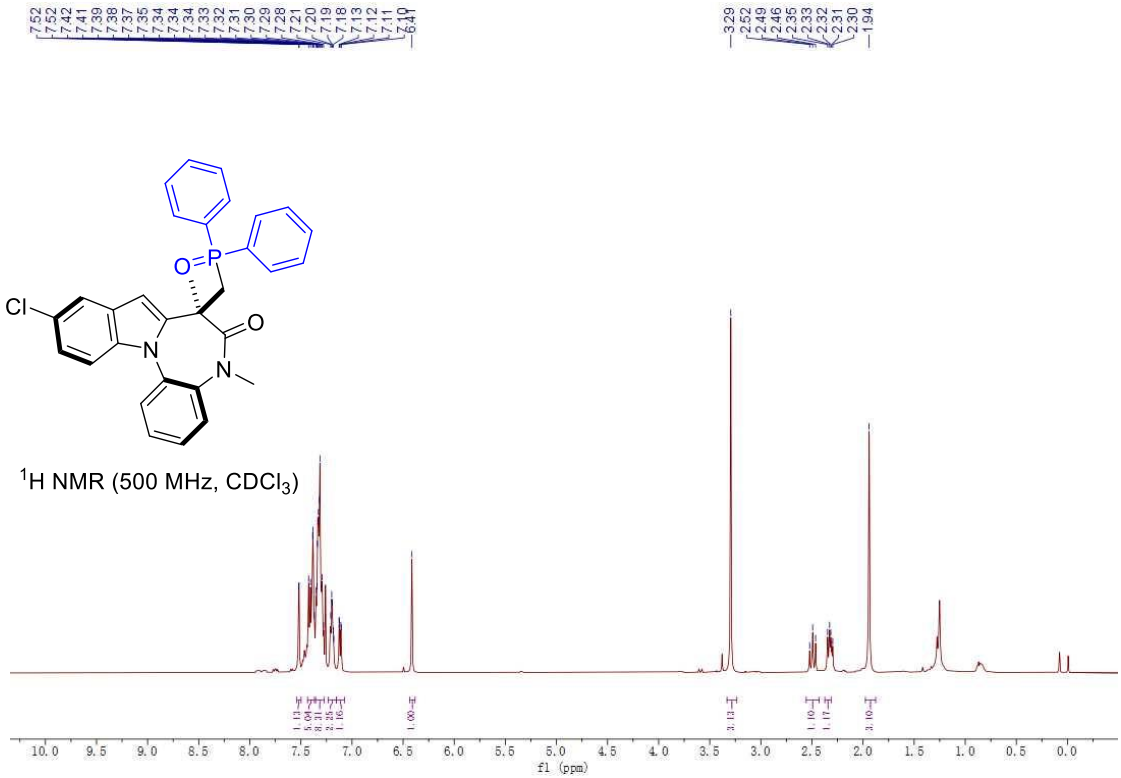
^{31}P NMR (202 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-5,7,11-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3f)

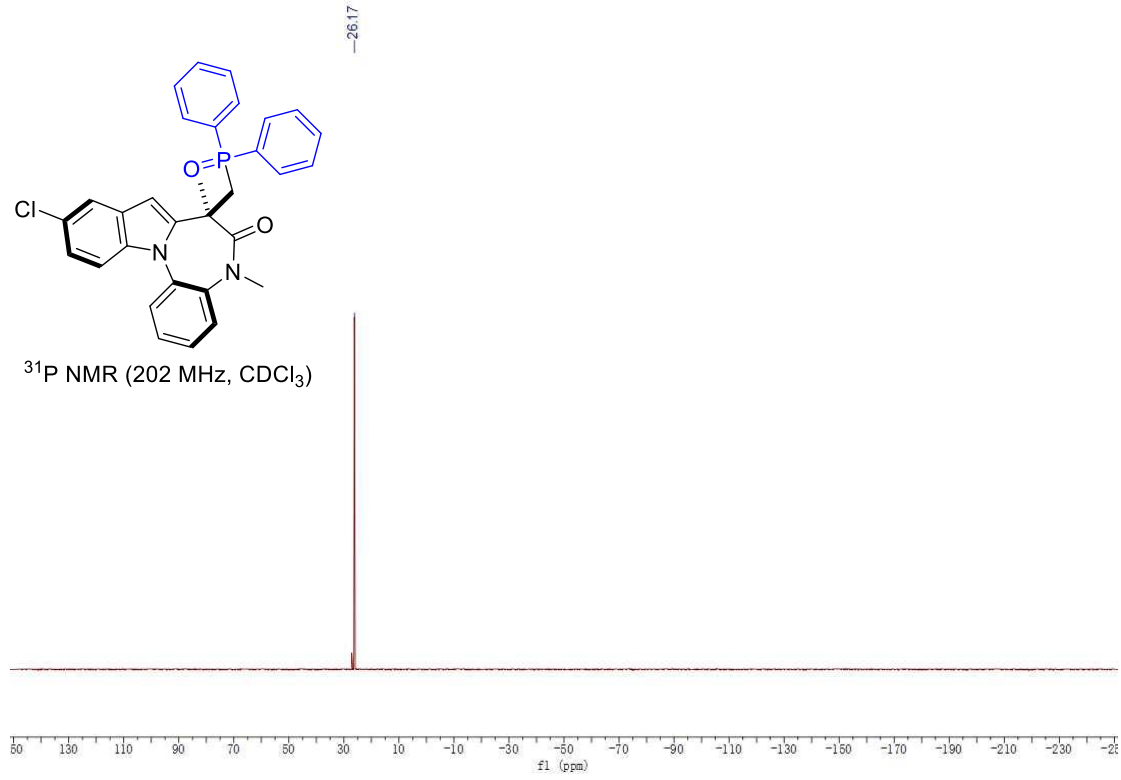


^{13}C NMR (126 MHz, $CDCl_3$)

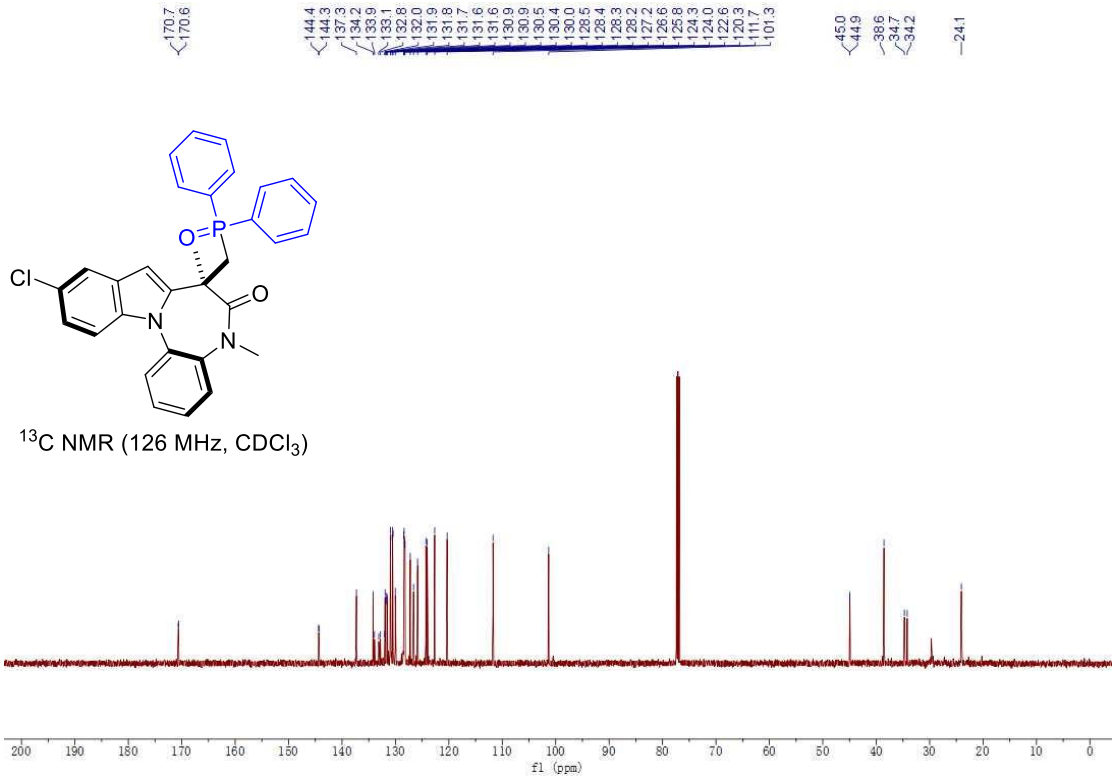
10-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3g)



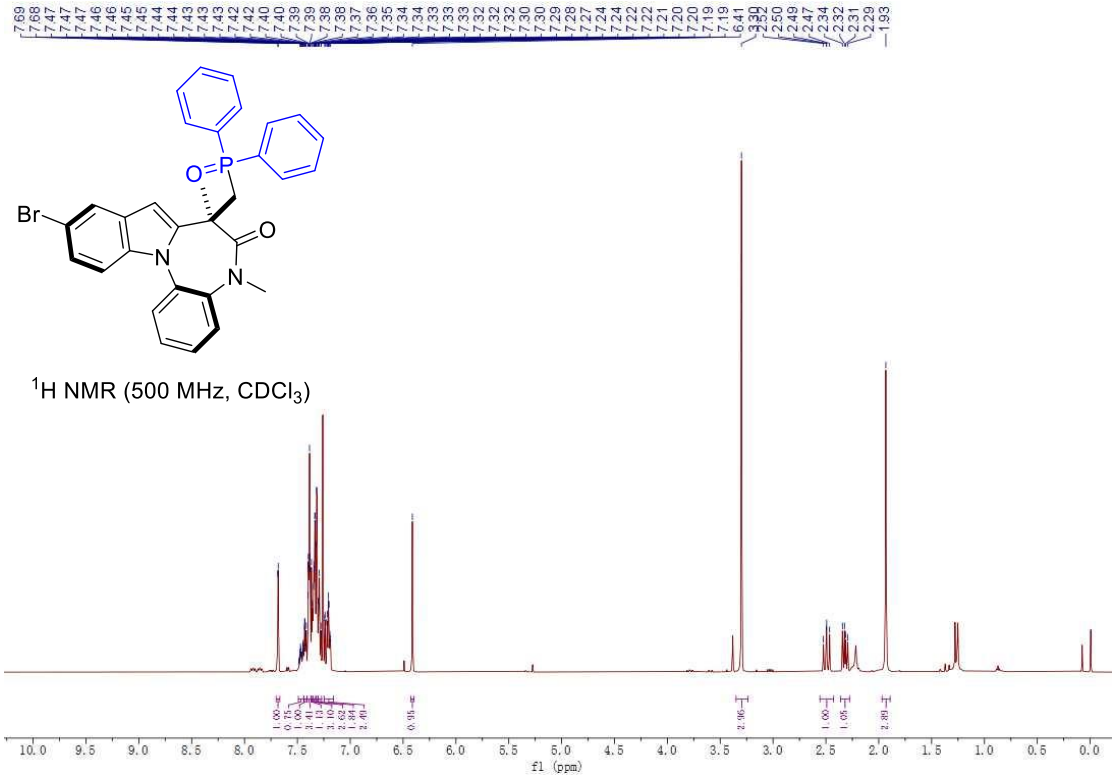
10-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3g)



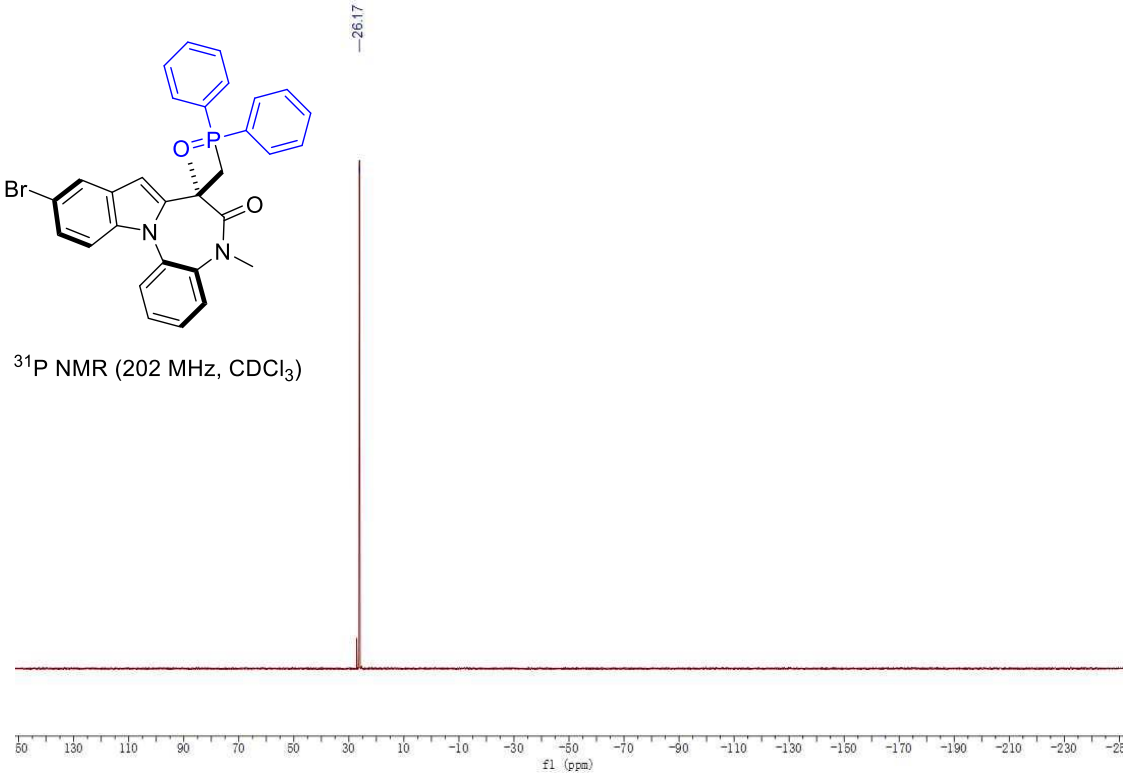
10-chloro-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3g)



10-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3h)

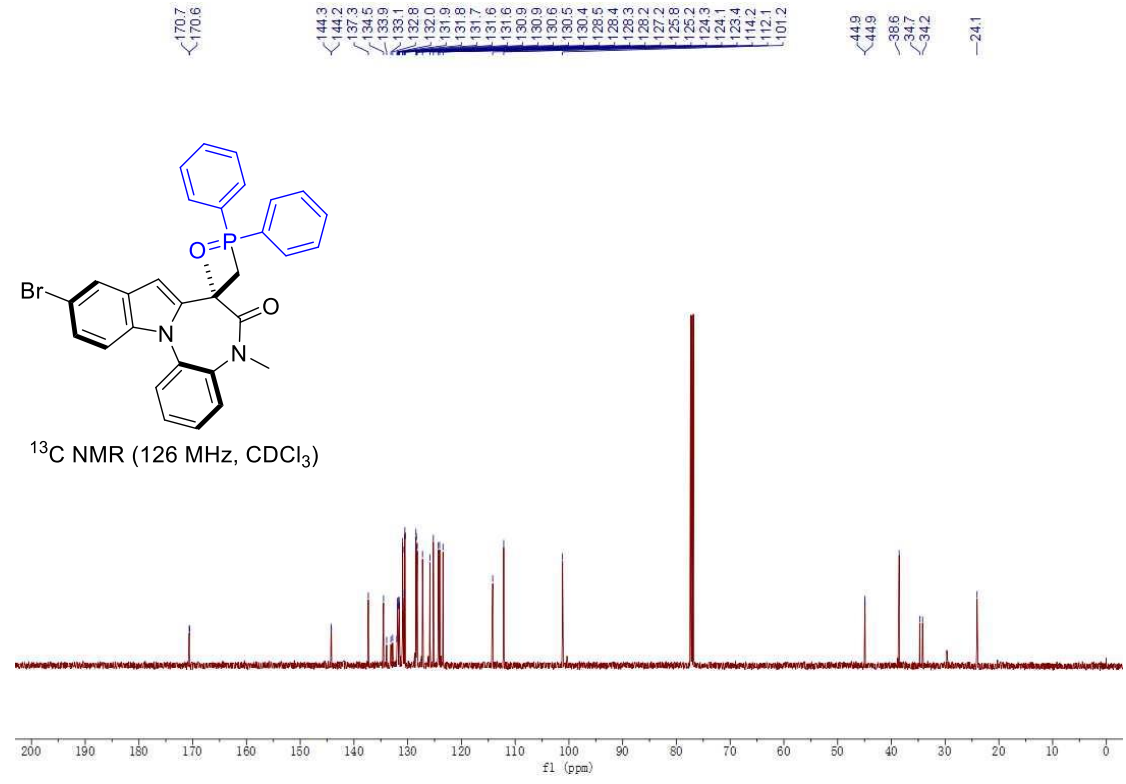


10-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3h)



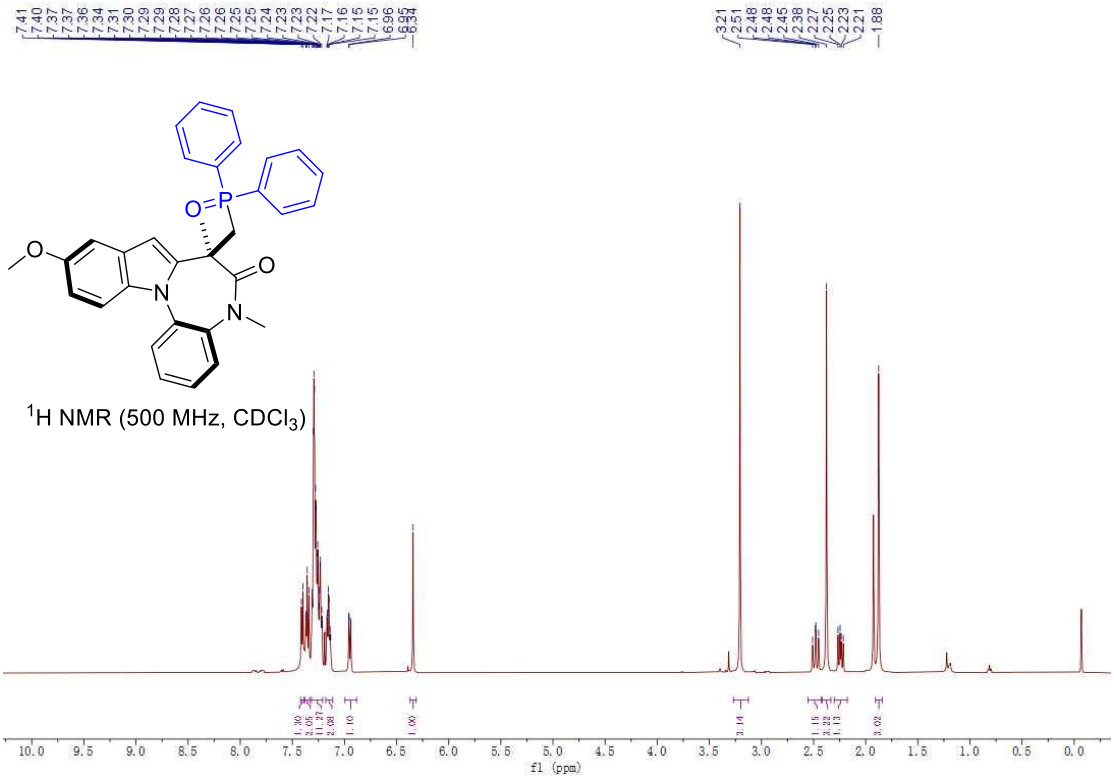
^{31}P NMR (202 MHz, $CDCl_3$)

10-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3h)

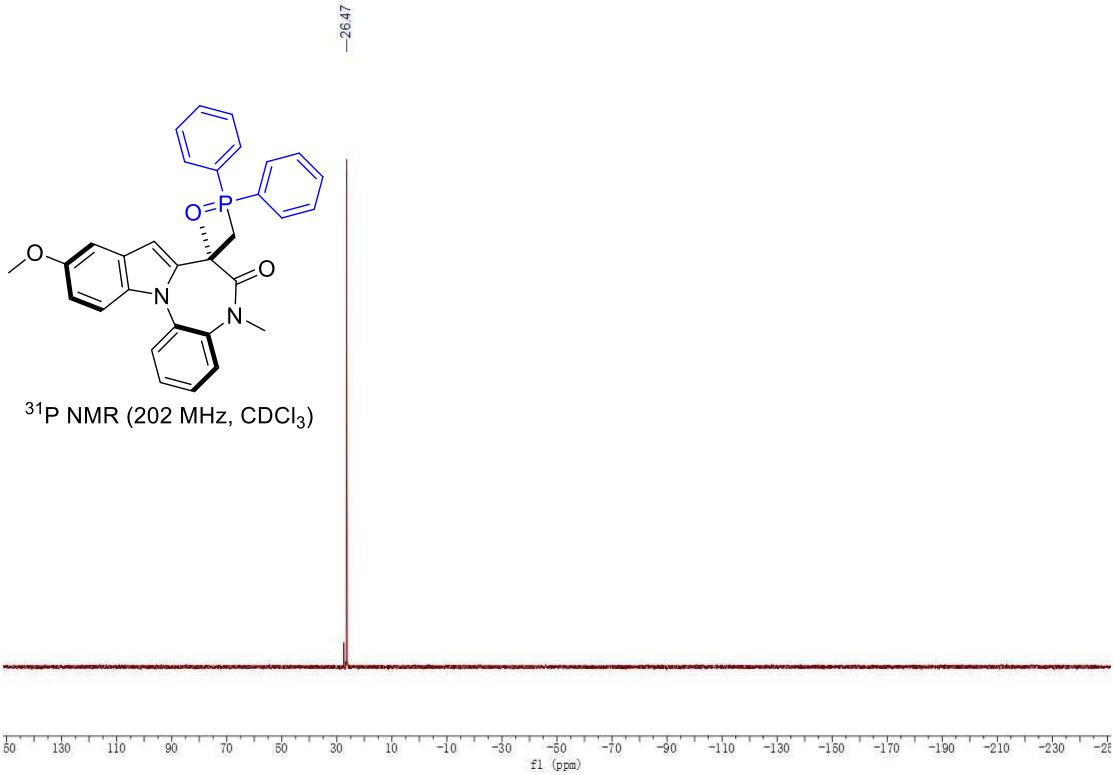


^{13}C NMR (126 MHz, $CDCl_3$)

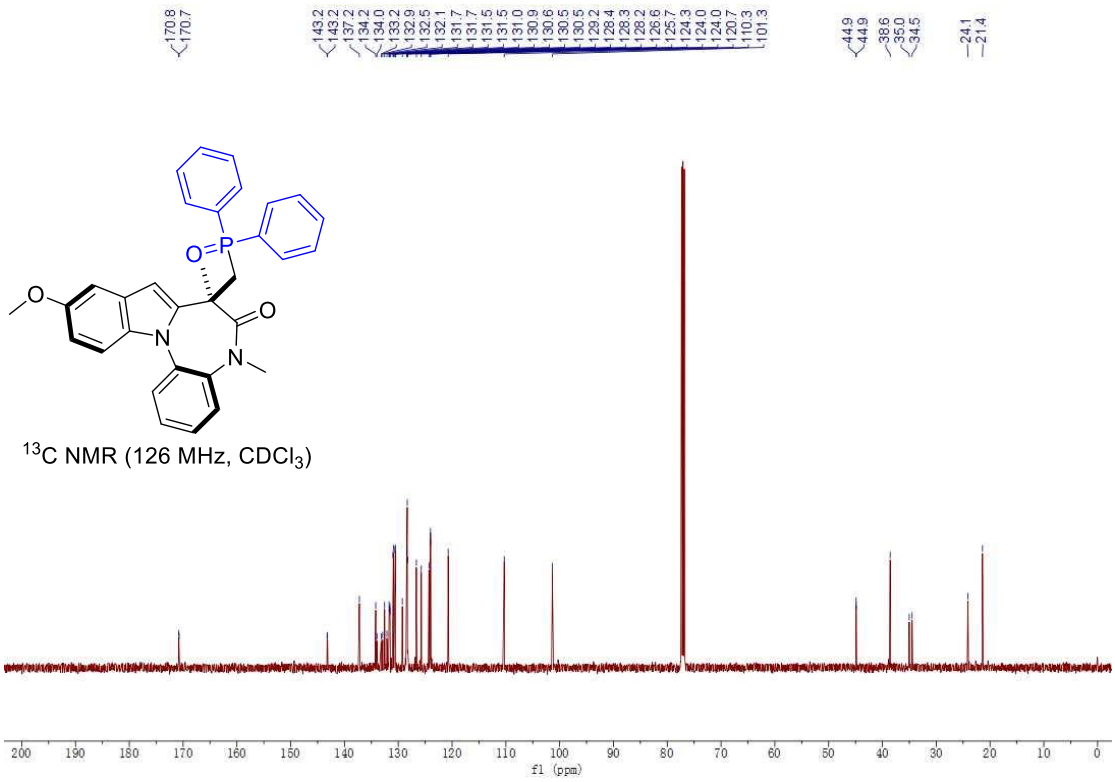
7-((diphenylphosphoryl)methyl)-10-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3i)



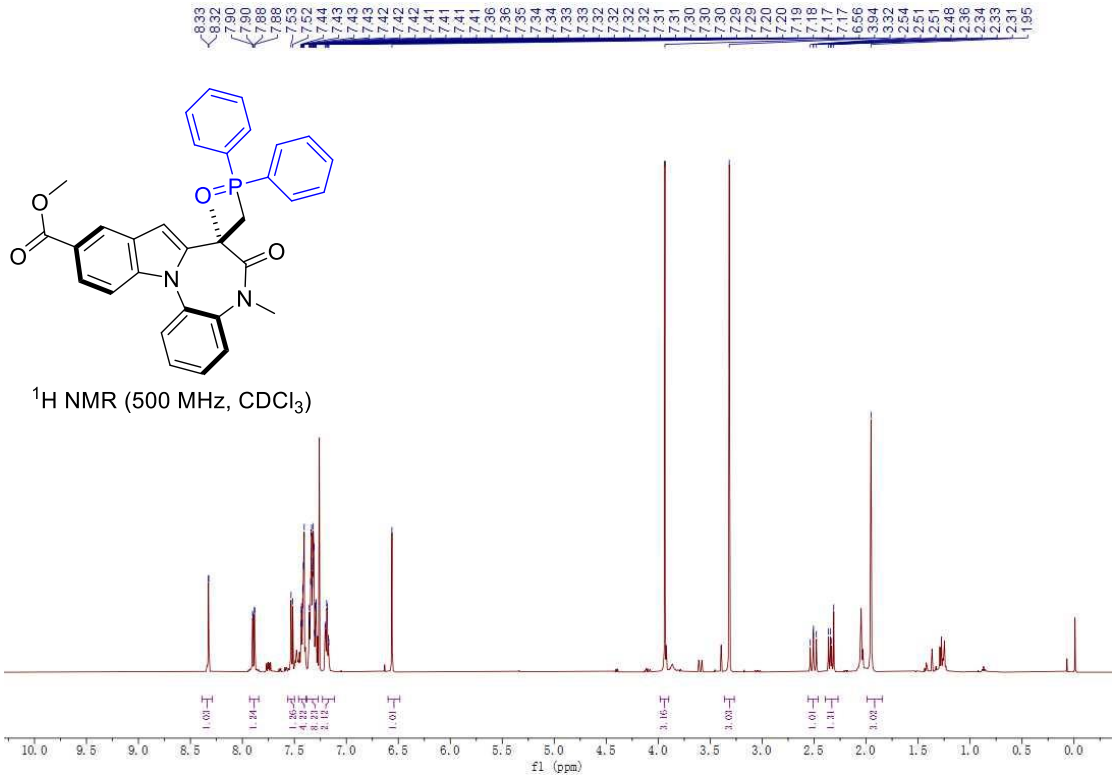
7-((diphenylphosphoryl)methyl)-10-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3i)



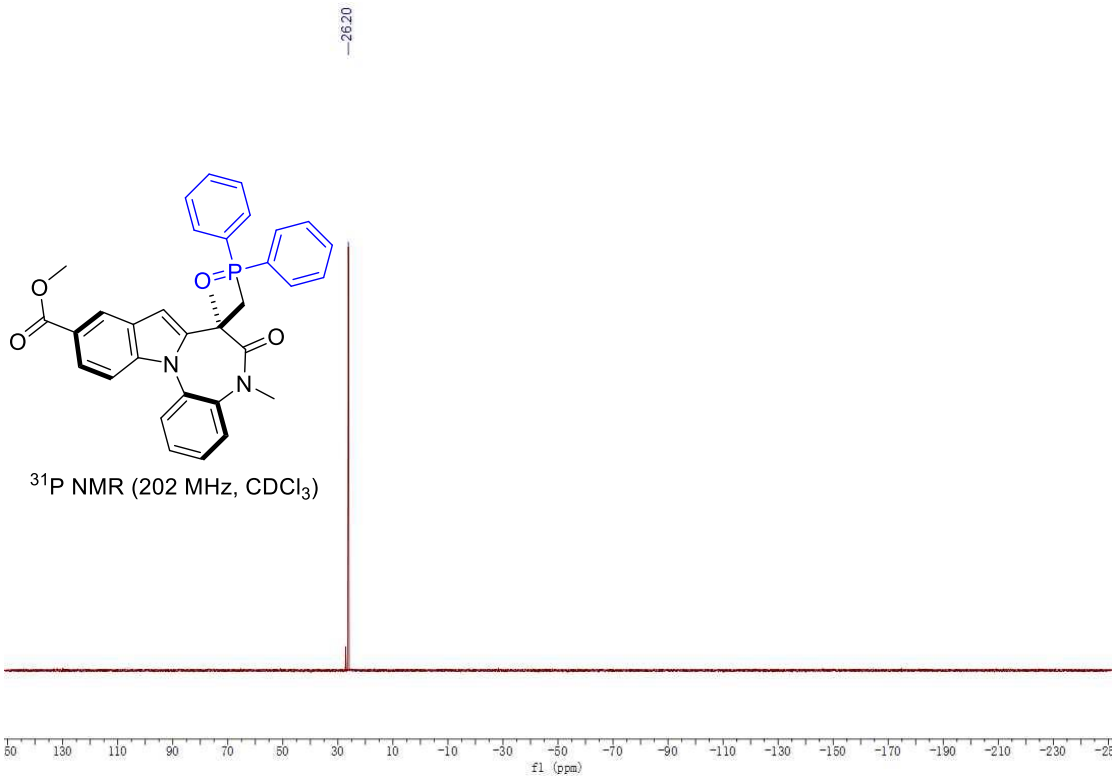
7-((diphenylphosphoryl)methyl)-10-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3i)



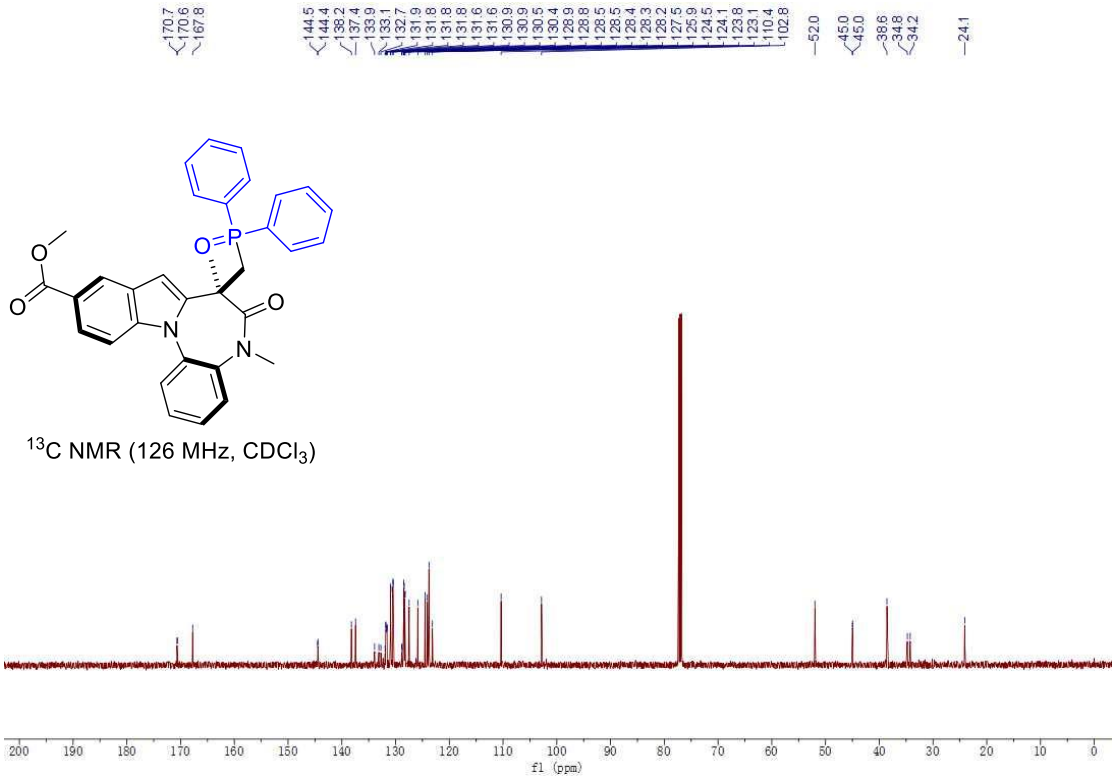
methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-10-carboxylate (3j)



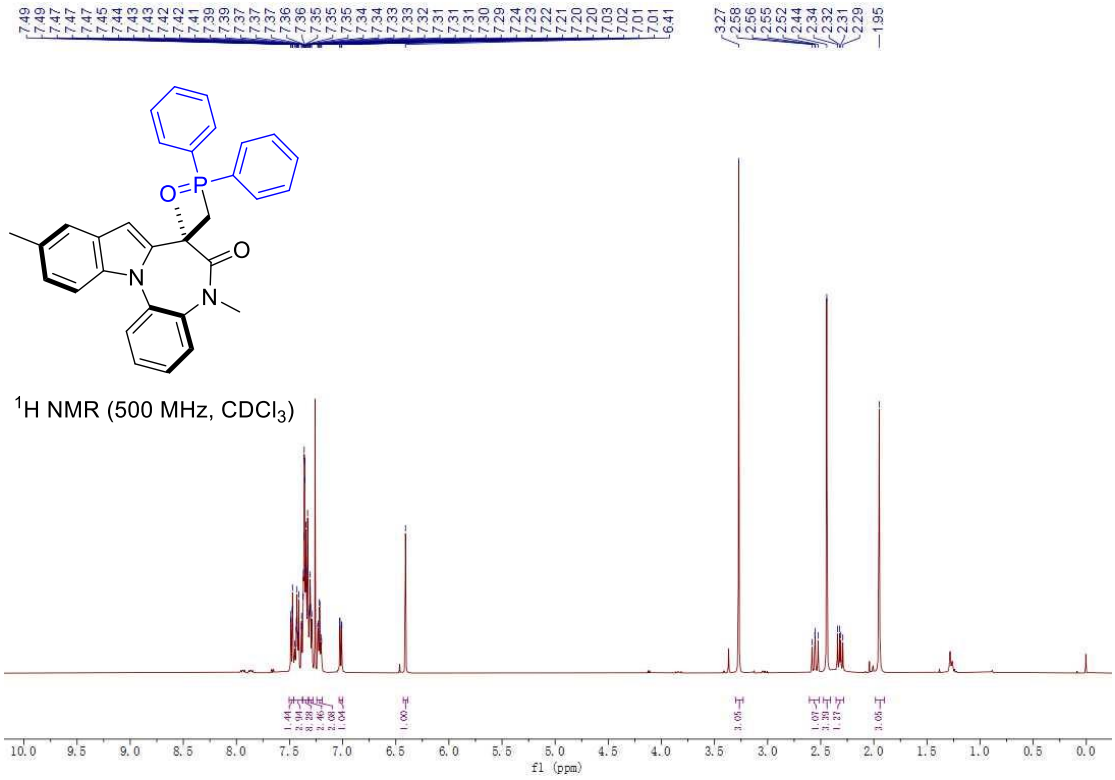
methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-10-carboxylate (3j)



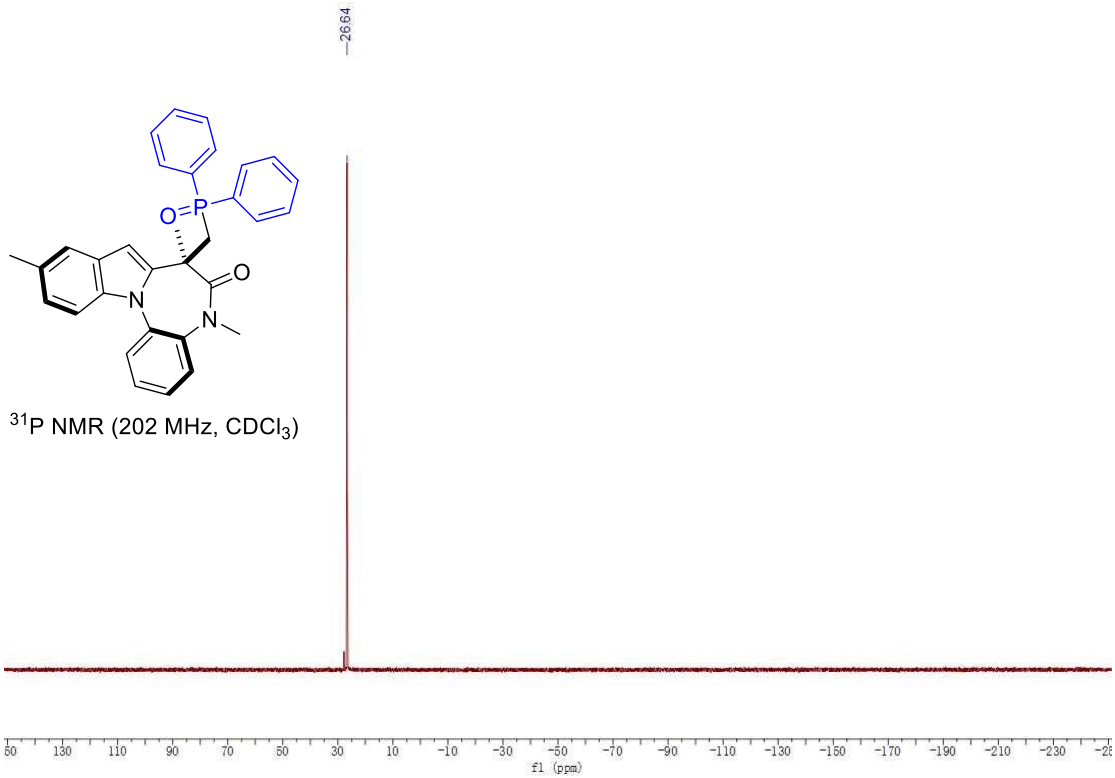
methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-10-carboxylate (3j)



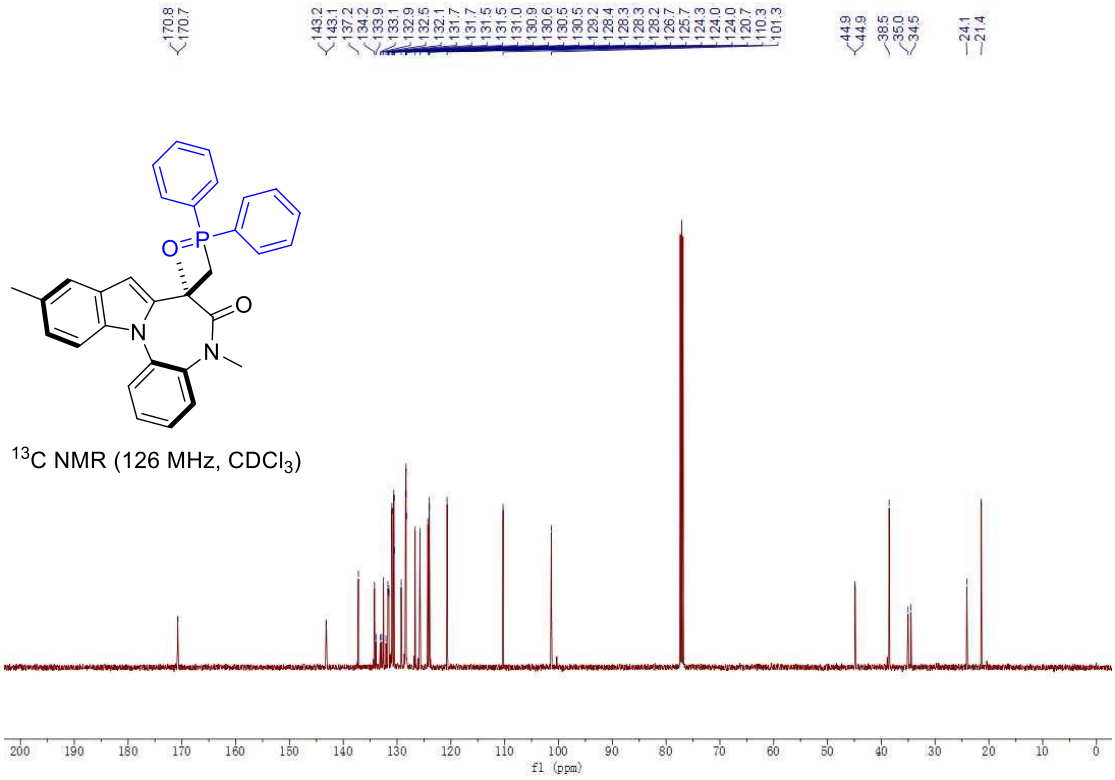
7-((diphenylphosphoryl)methyl)-5,7,10-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3k)



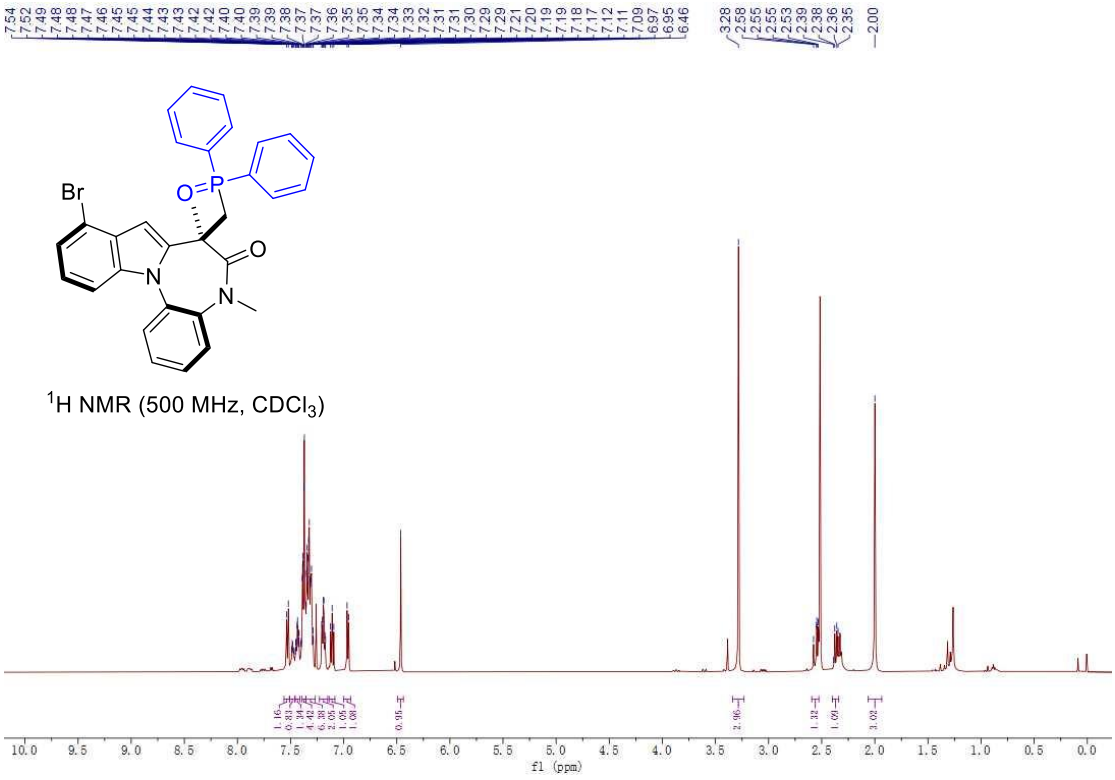
7-((diphenylphosphoryl)methyl)-5,7,10-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3k)



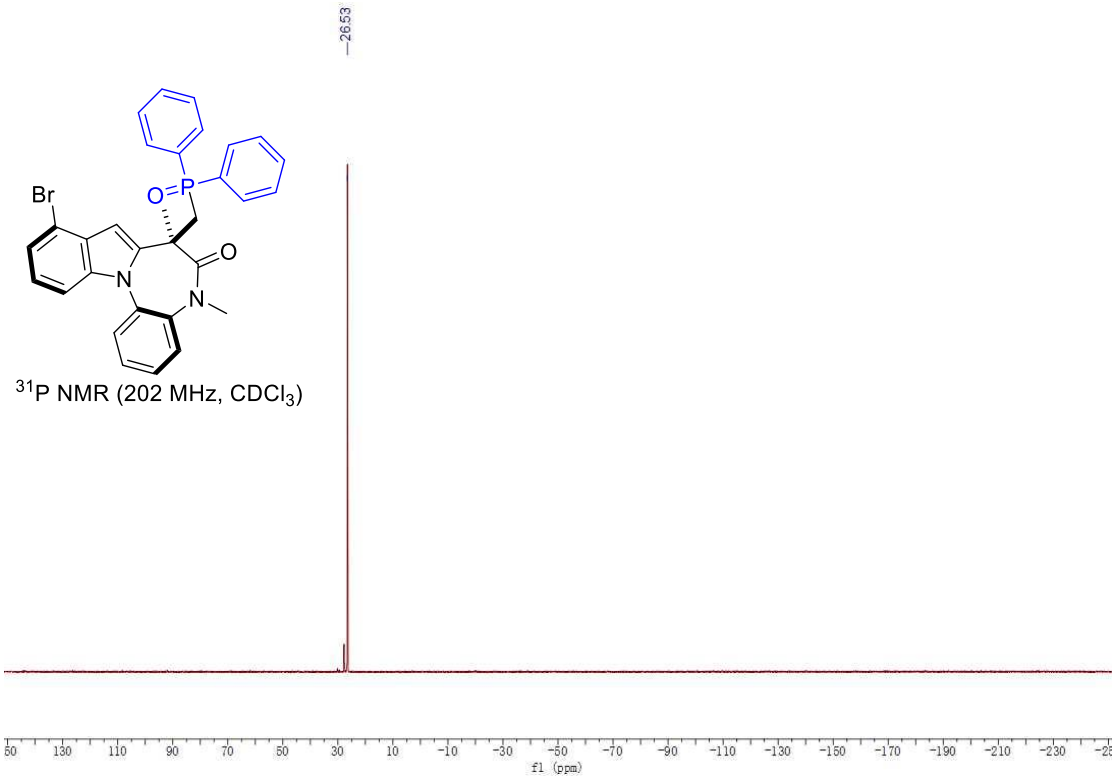
7-((diphenylphosphoryl)methyl)-5,7,10-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3k)



9-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3l)

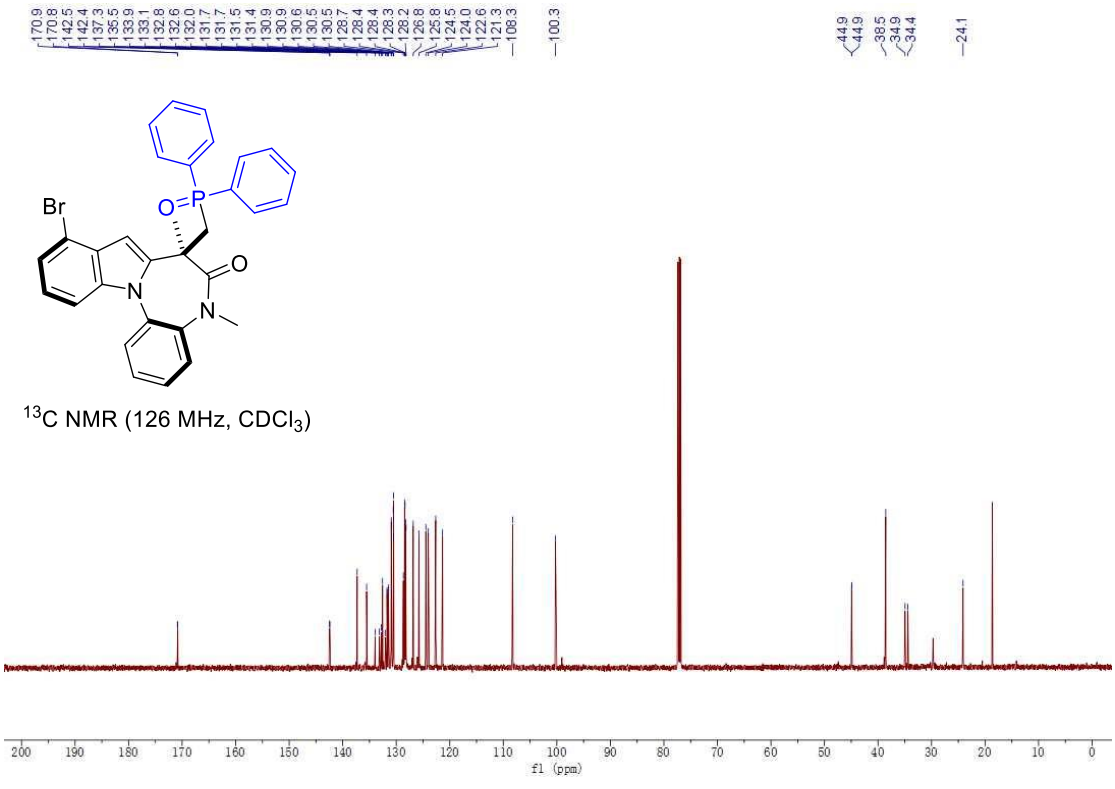


9-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3l)



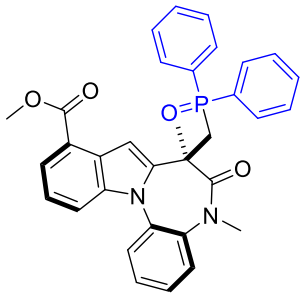
^{31}P NMR (202 MHz, $CDCl_3$)

9-bromo-7-((diphenylphosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3l)

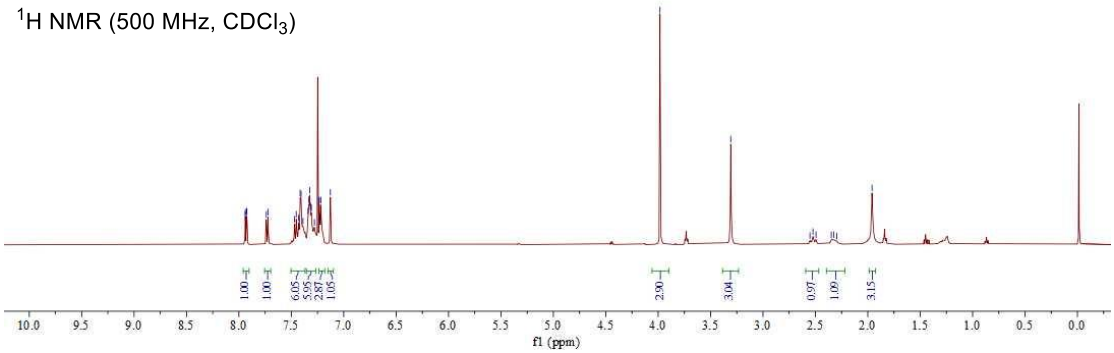


^{13}C NMR (126 MHz, $CDCl_3$)

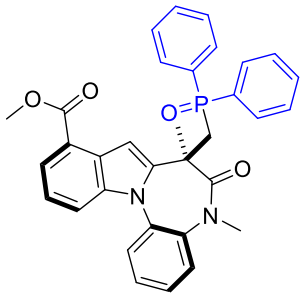
methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-9-carboxylate (3m)



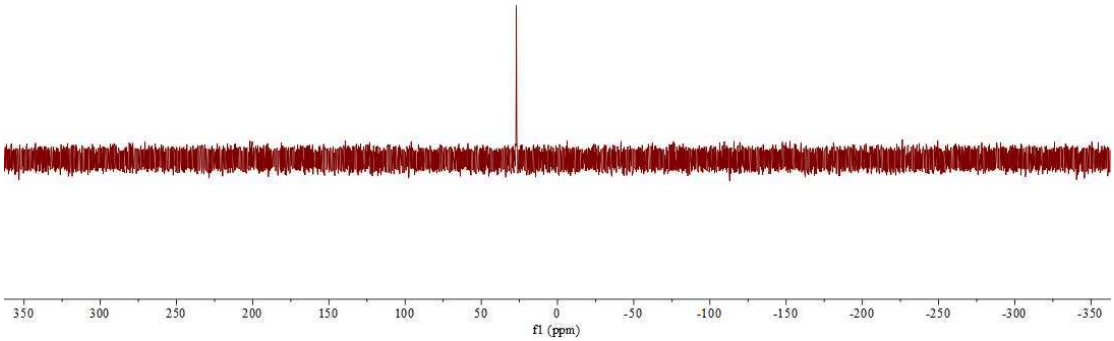
^{1}H NMR (500 MHz, $CDCl_3$)



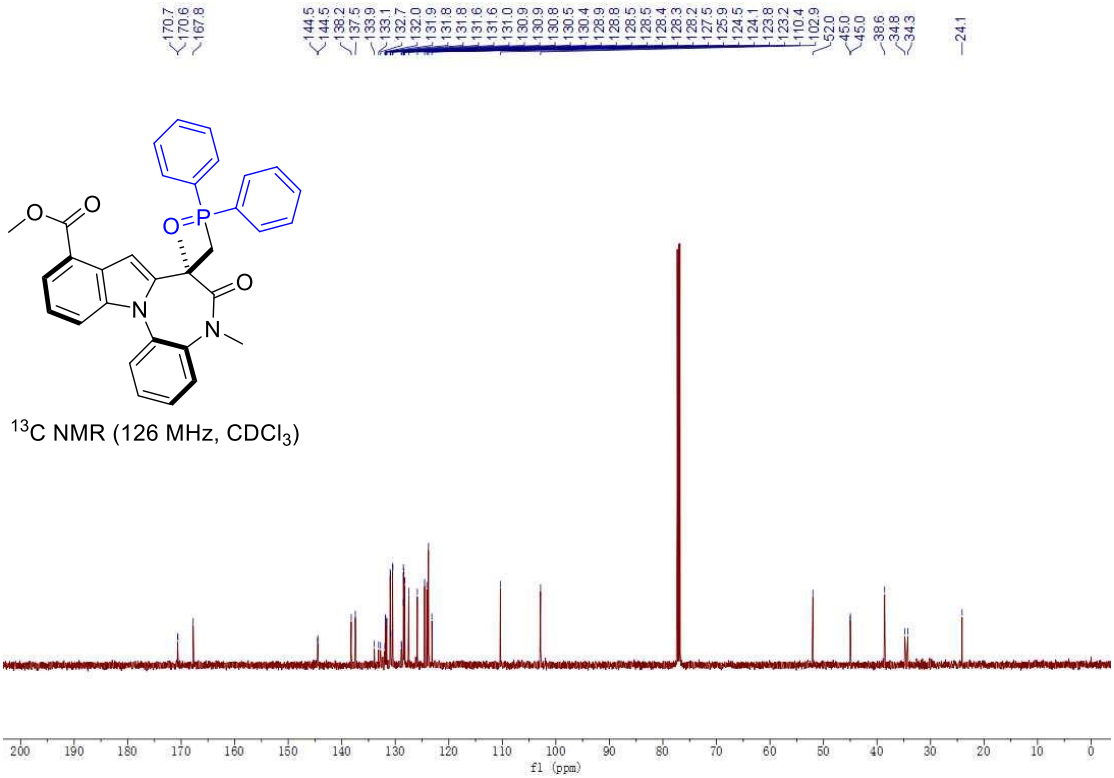
methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-9-carboxylate (3m)



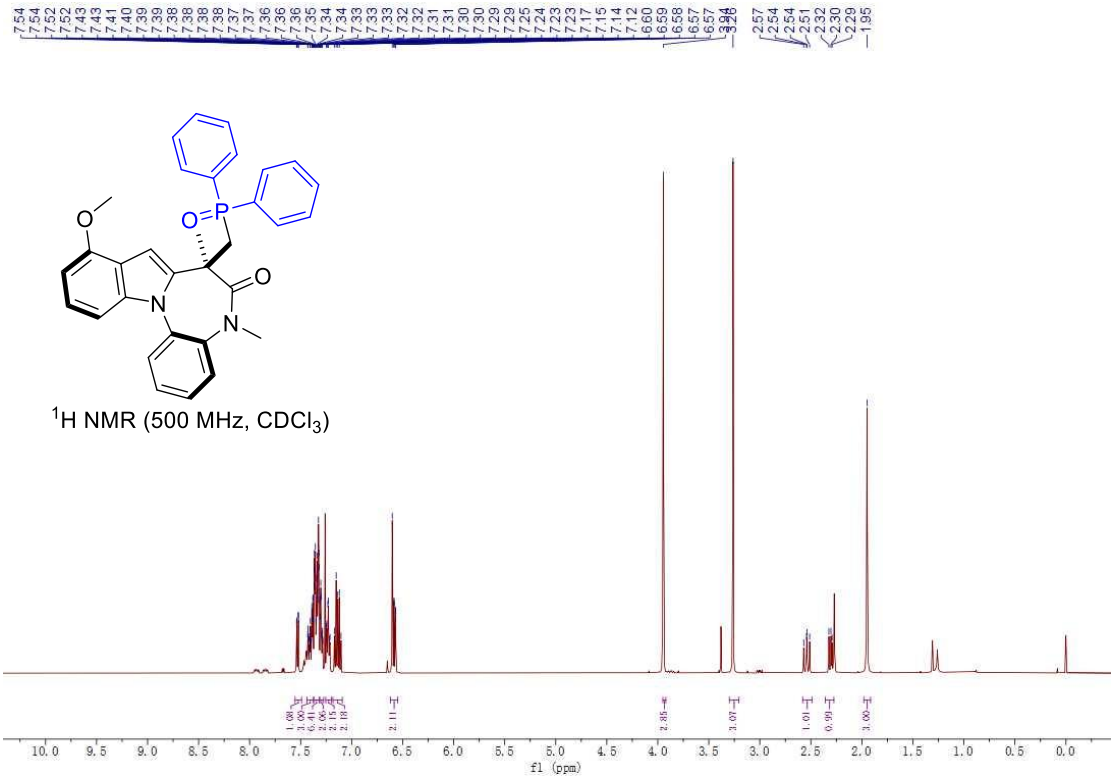
^{31}P NMR (202 MHz, $CDCl_3$)



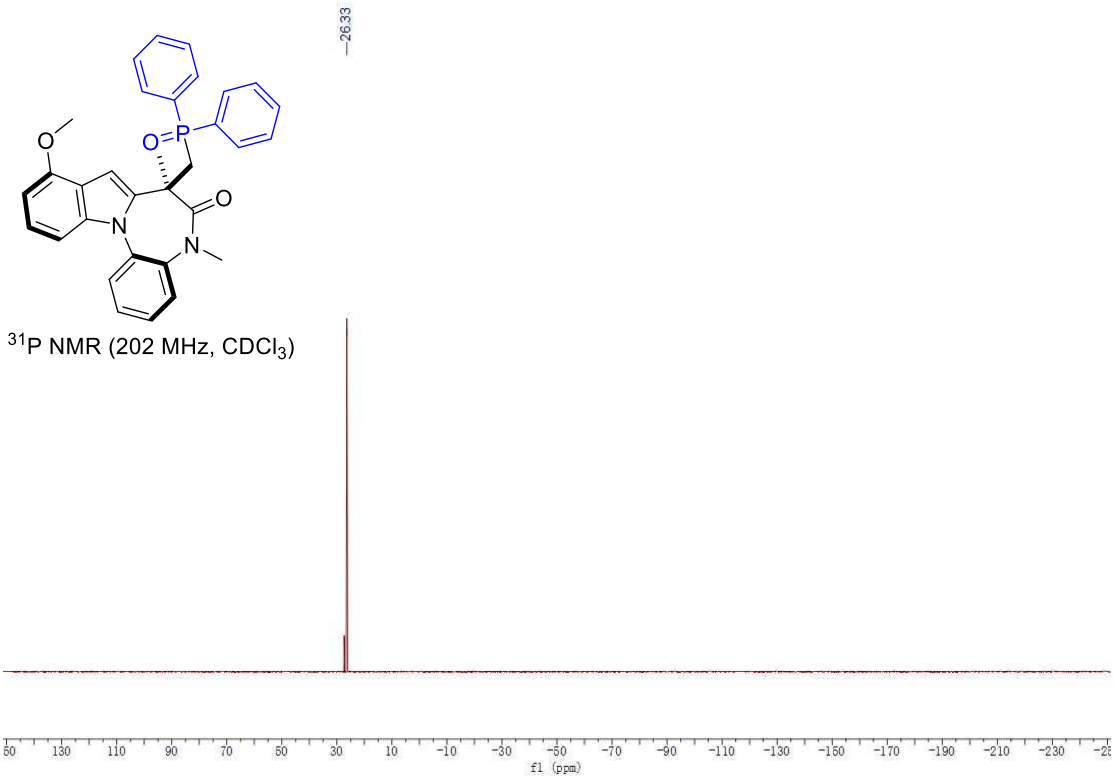
methyl 7-((diphenylphosphoryl)methyl)-5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indole-9-carboxylate (3m)



7-((diphenylphosphoryl)methyl)-9-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3n)

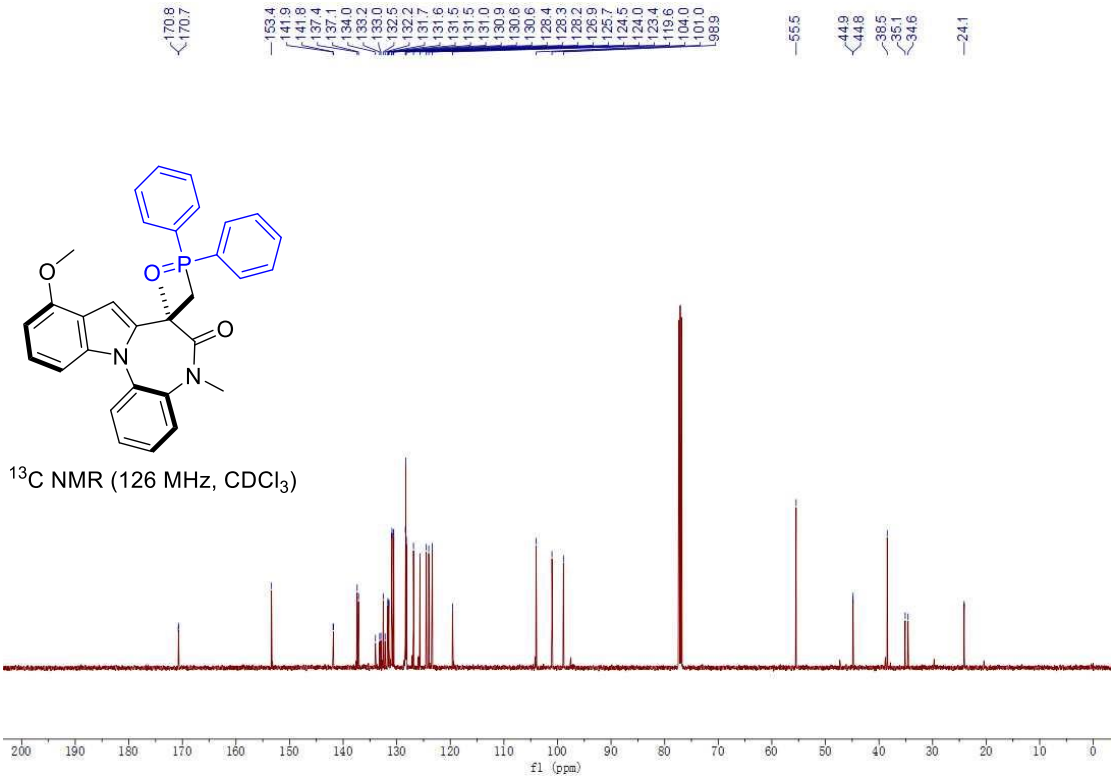


7-((diphenylphosphoryl)methyl)-9-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3n)



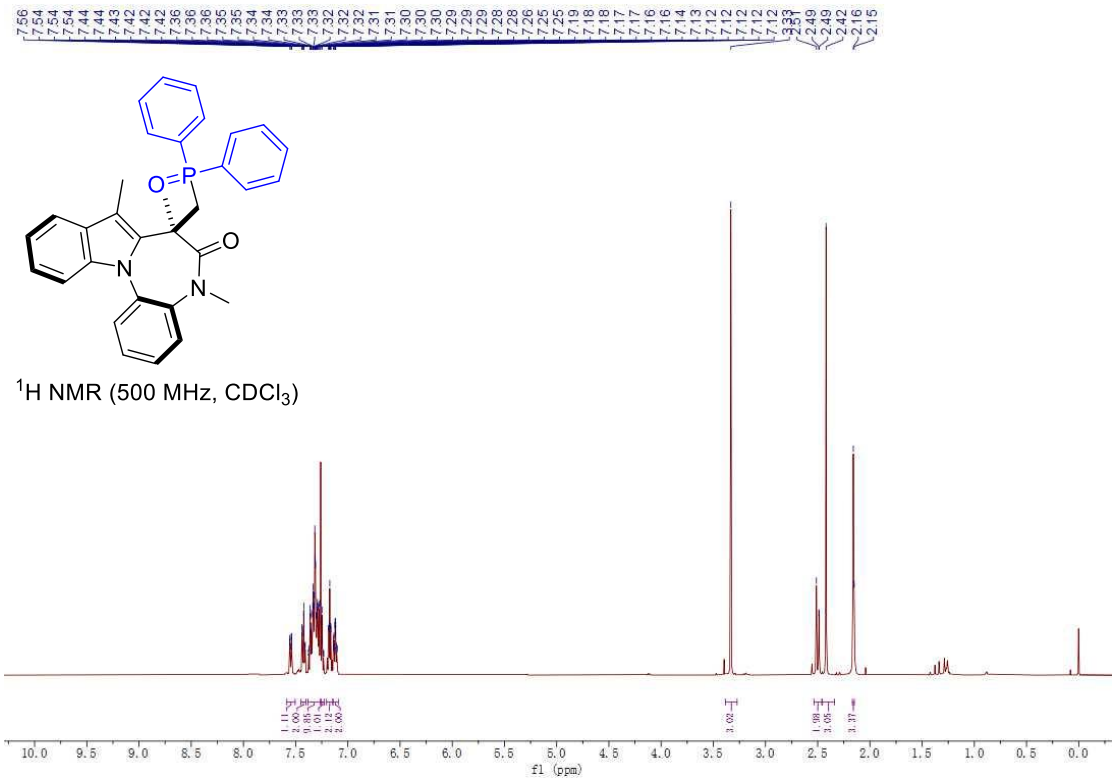
^{31}P NMR (202 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-9-methoxy-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3n)

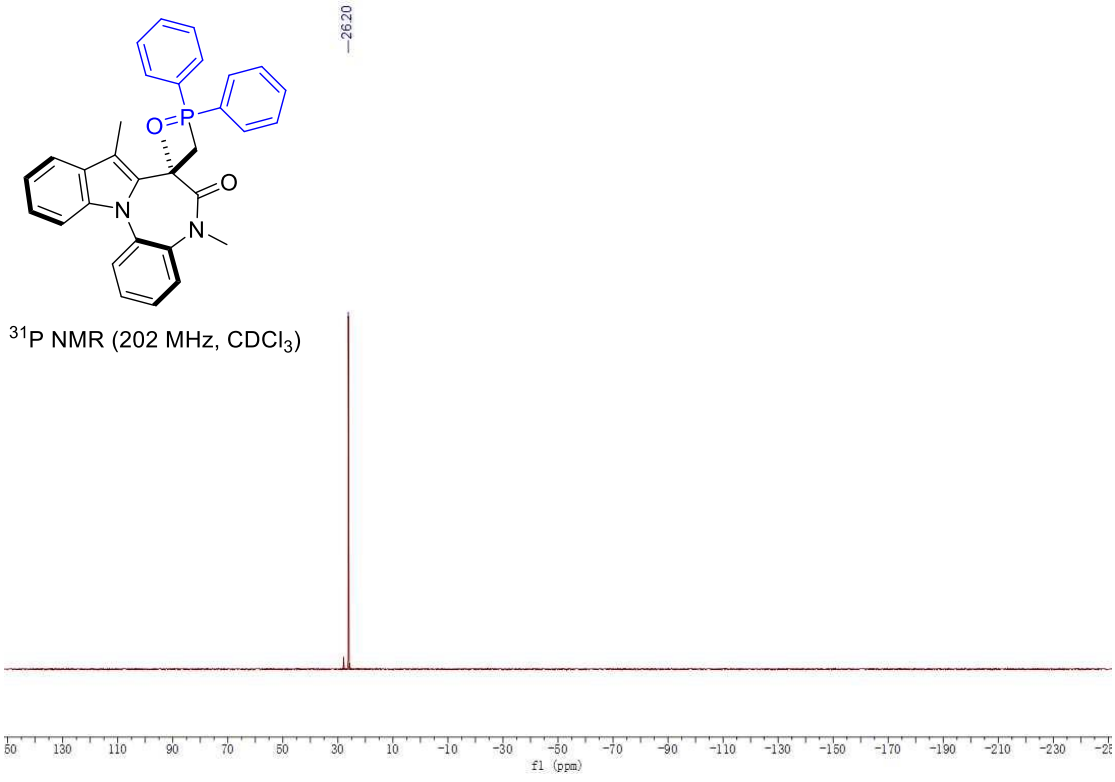


^{13}C NMR (126 MHz, $CDCl_3$)

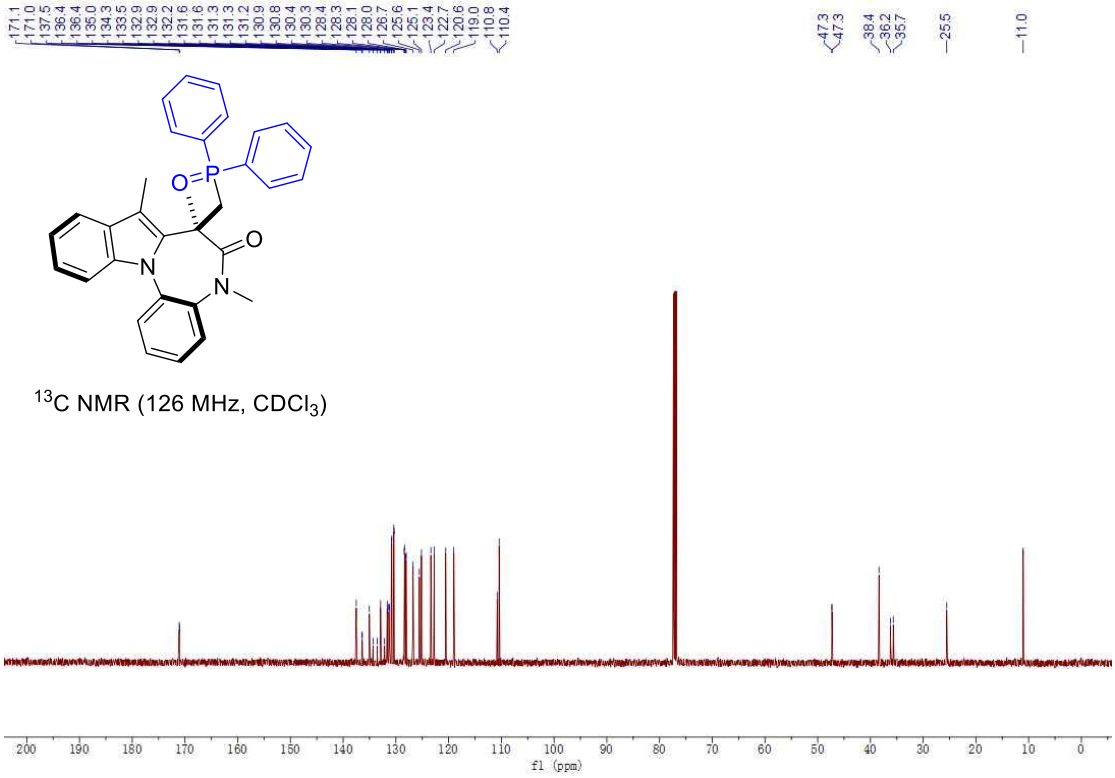
7-((diphenylphosphoryl)methyl)-5,7,8-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3o)



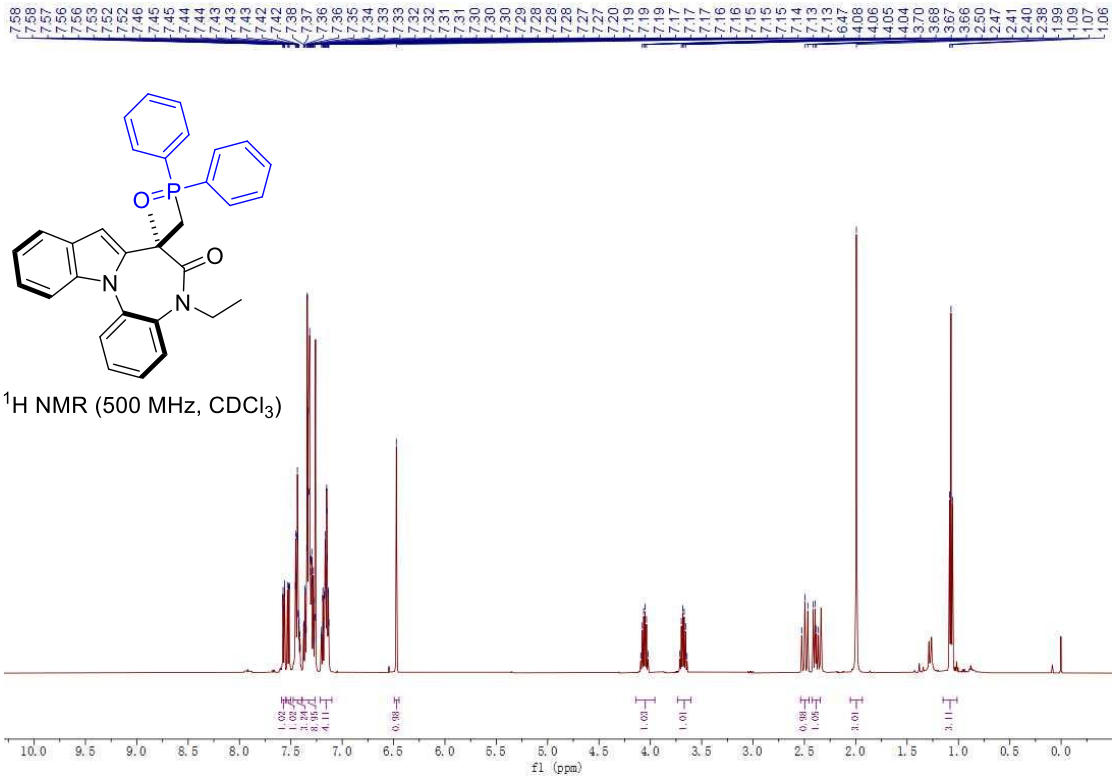
7-((diphenylphosphoryl)methyl)-5,7,8-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3o)



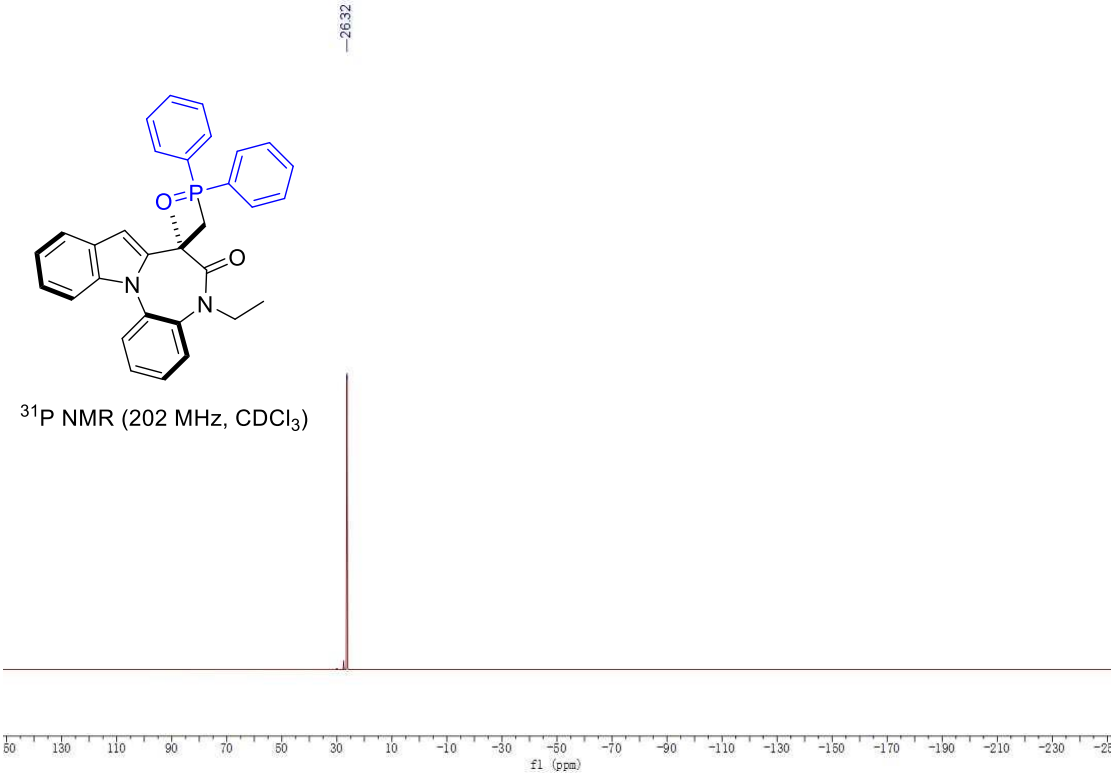
7-((diphenylphosphoryl)methyl)-5,7,8-trimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3o)



7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3p)

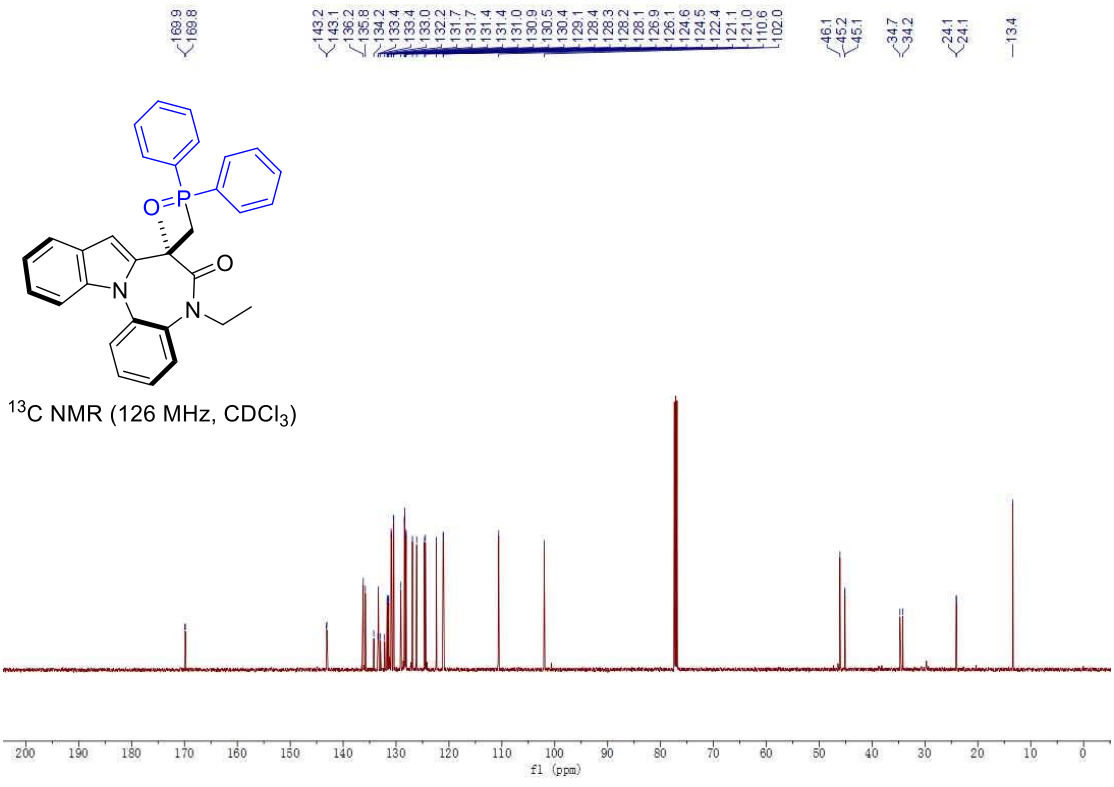


7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3p)



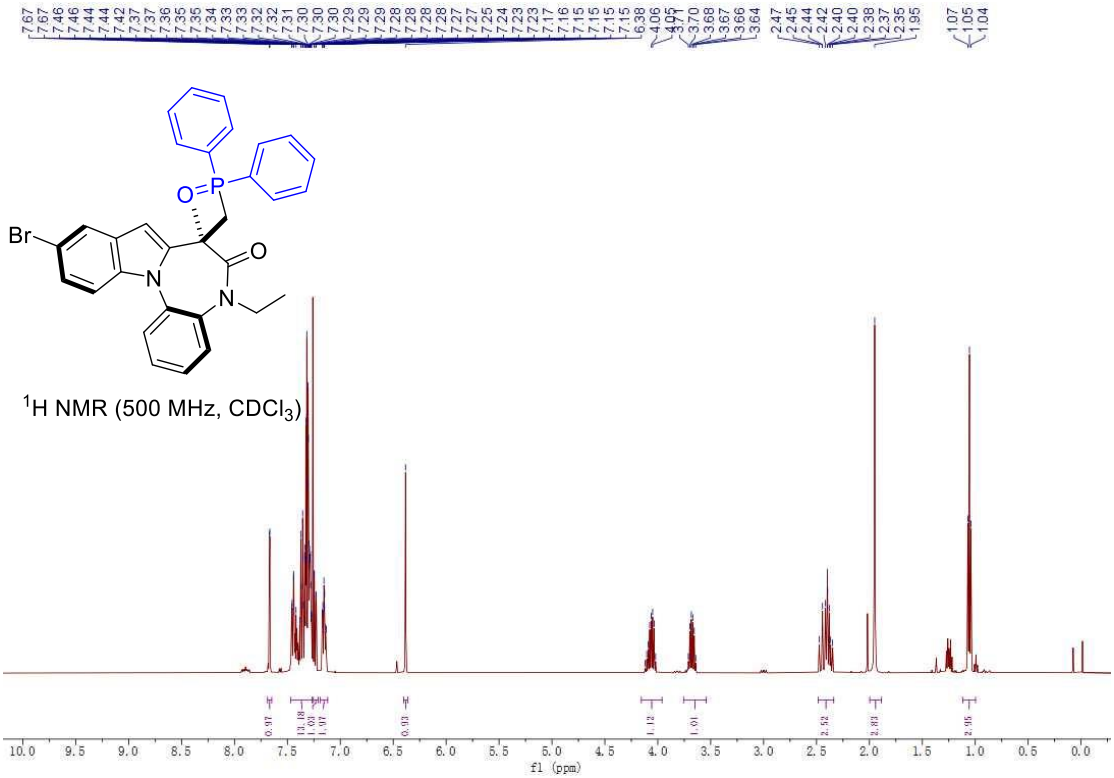
^{31}P NMR (202 MHz, $CDCl_3$)

7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3p)

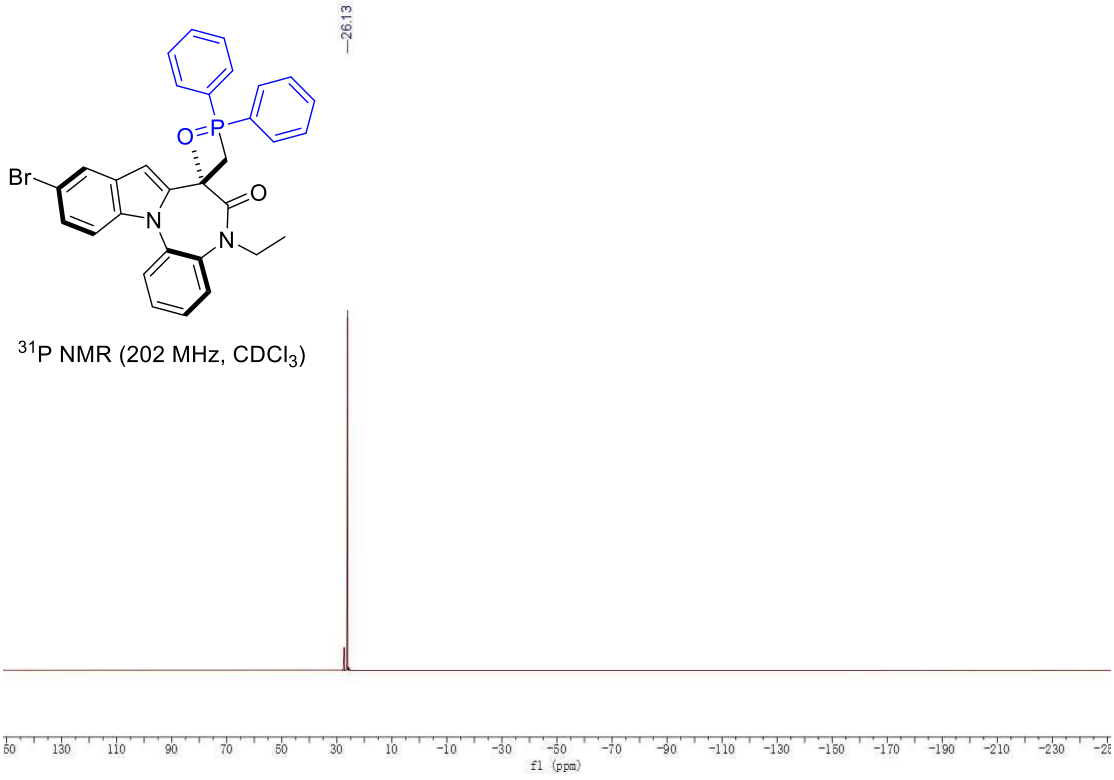


^{13}C NMR (126 MHz, $CDCl_3$)

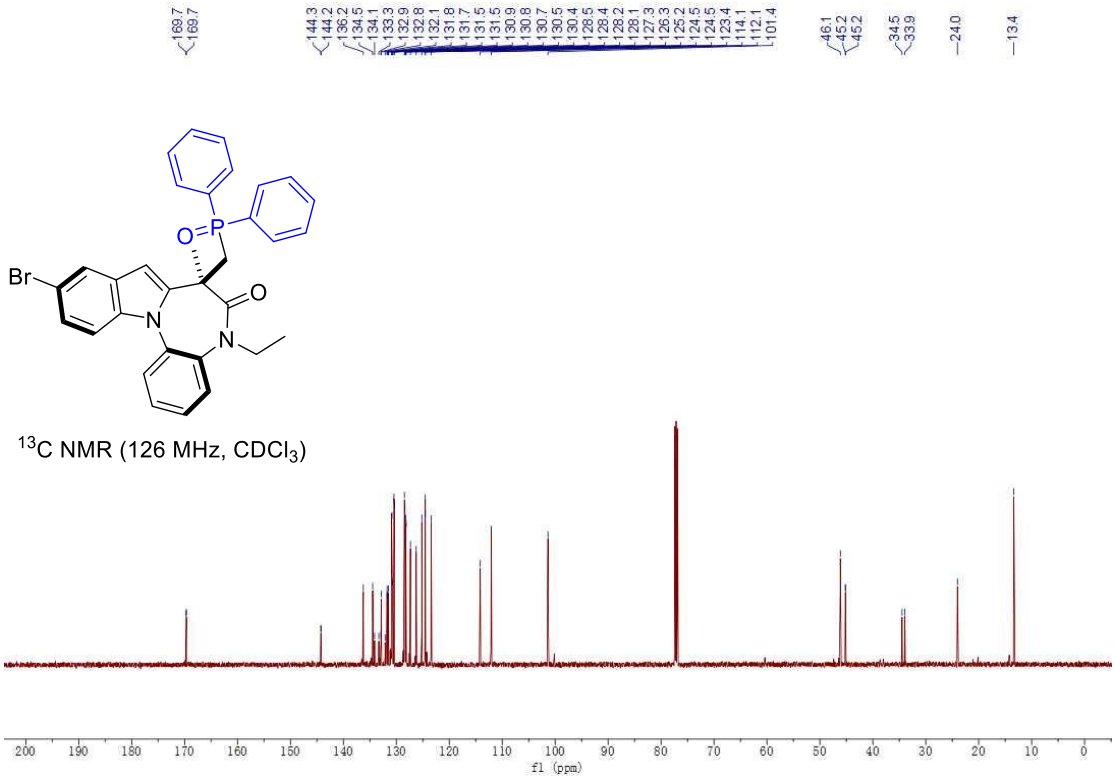
10-bromo-7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3q)



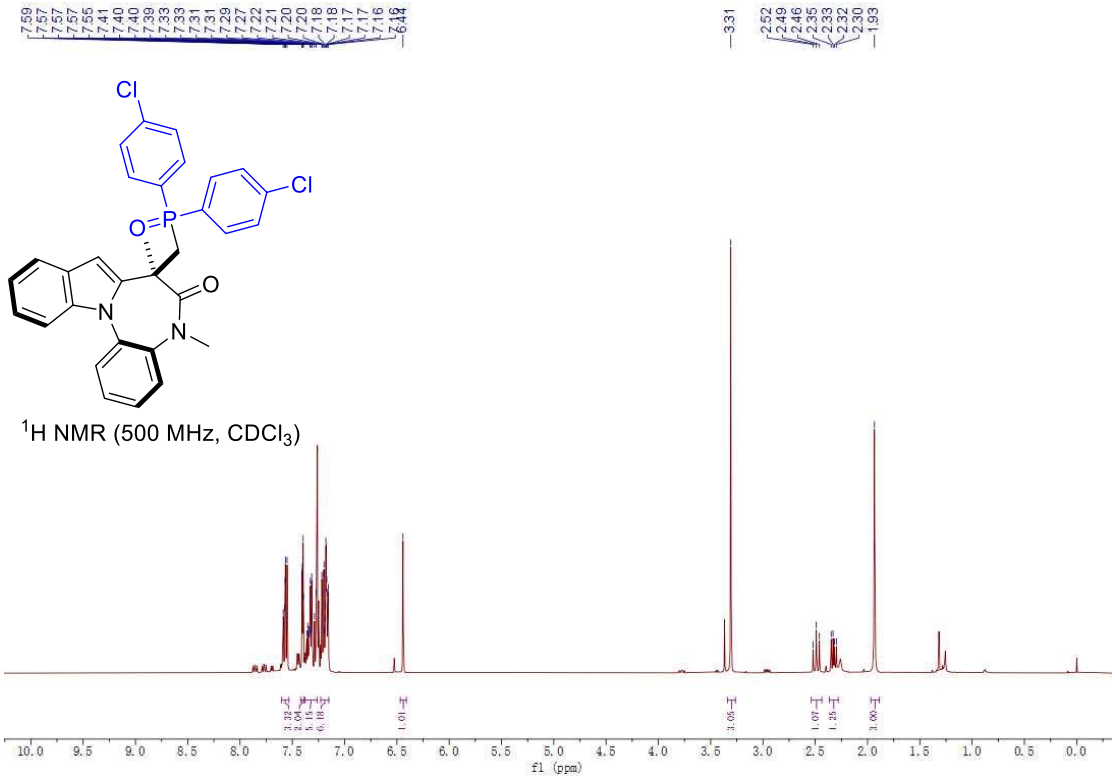
10-bromo-7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3q)



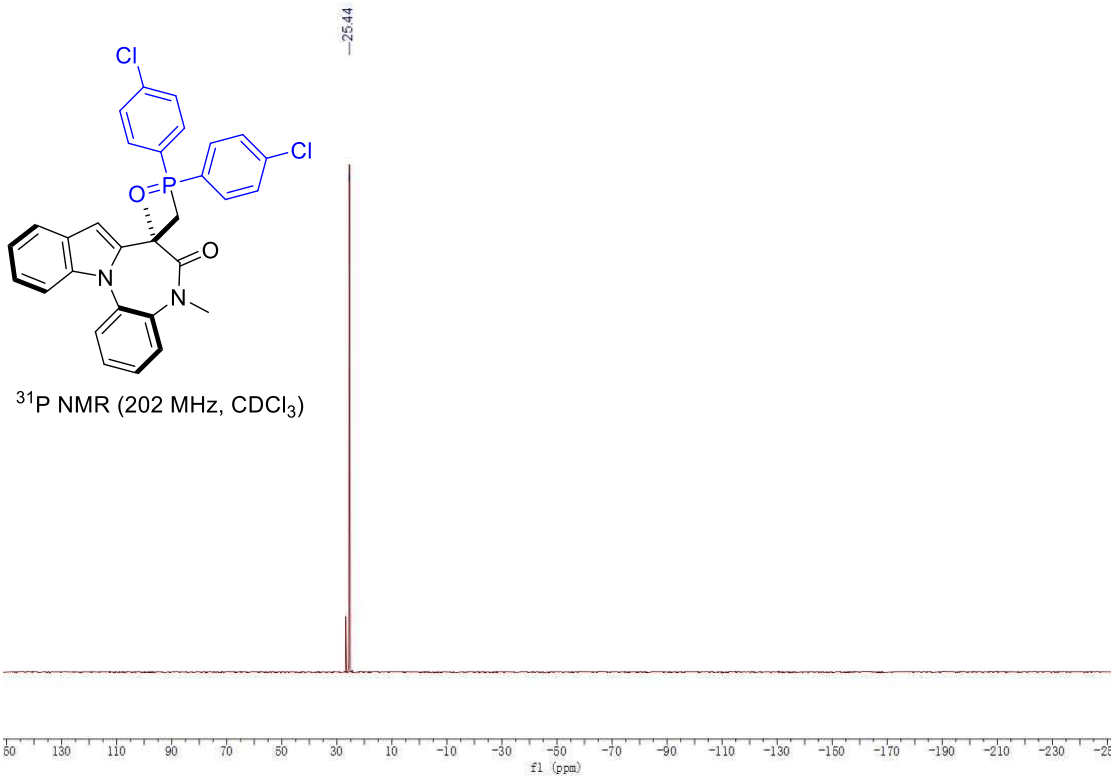
10-bromo-7-((diphenylphosphoryl)methyl)-5-ethyl-7-methyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3q)



7-((bis(4-chlorophenyl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3r)

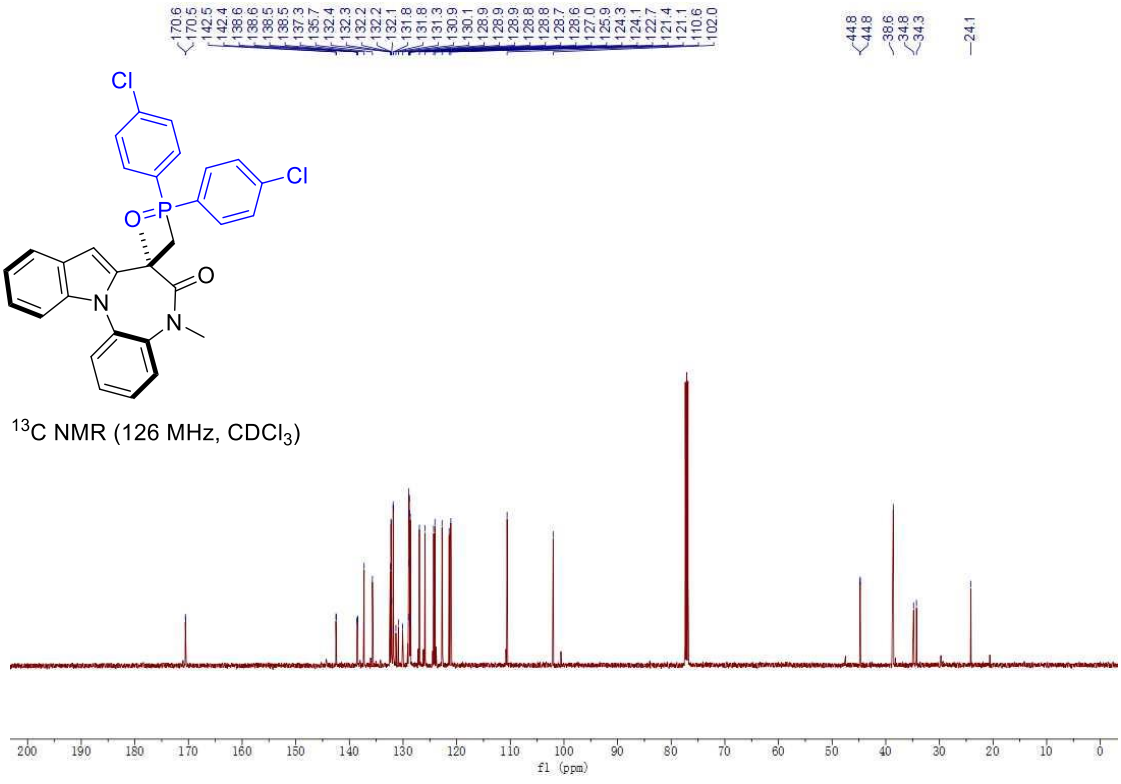


7-((bis(4-chlorophenyl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3r)



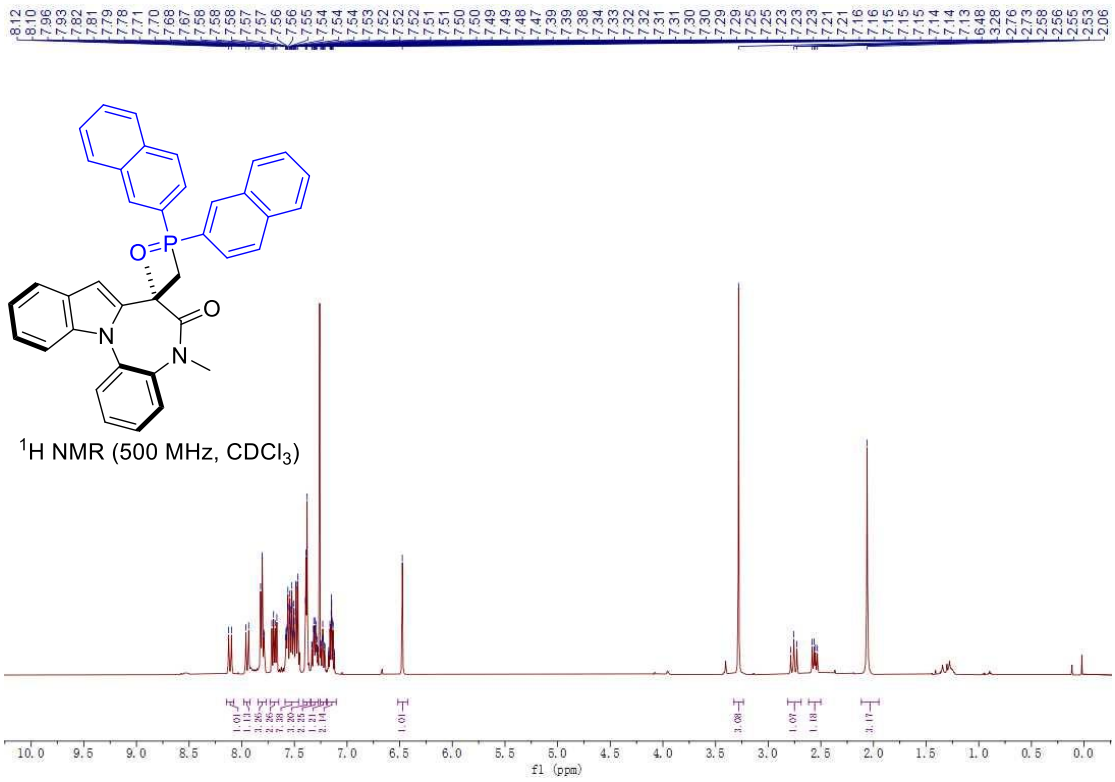
^{31}P NMR (202 MHz, $CDCl_3$)

7-((bis(4-chlorophenyl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3r)

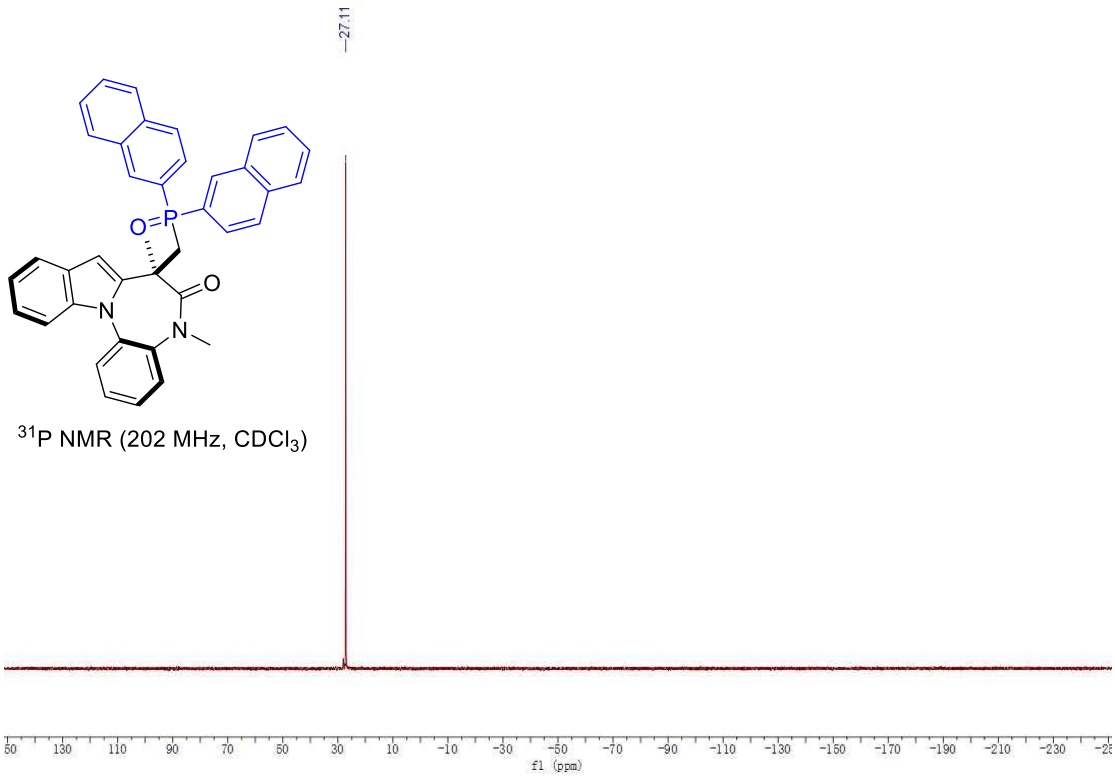


^{13}C NMR (126 MHz, $CDCl_3$)

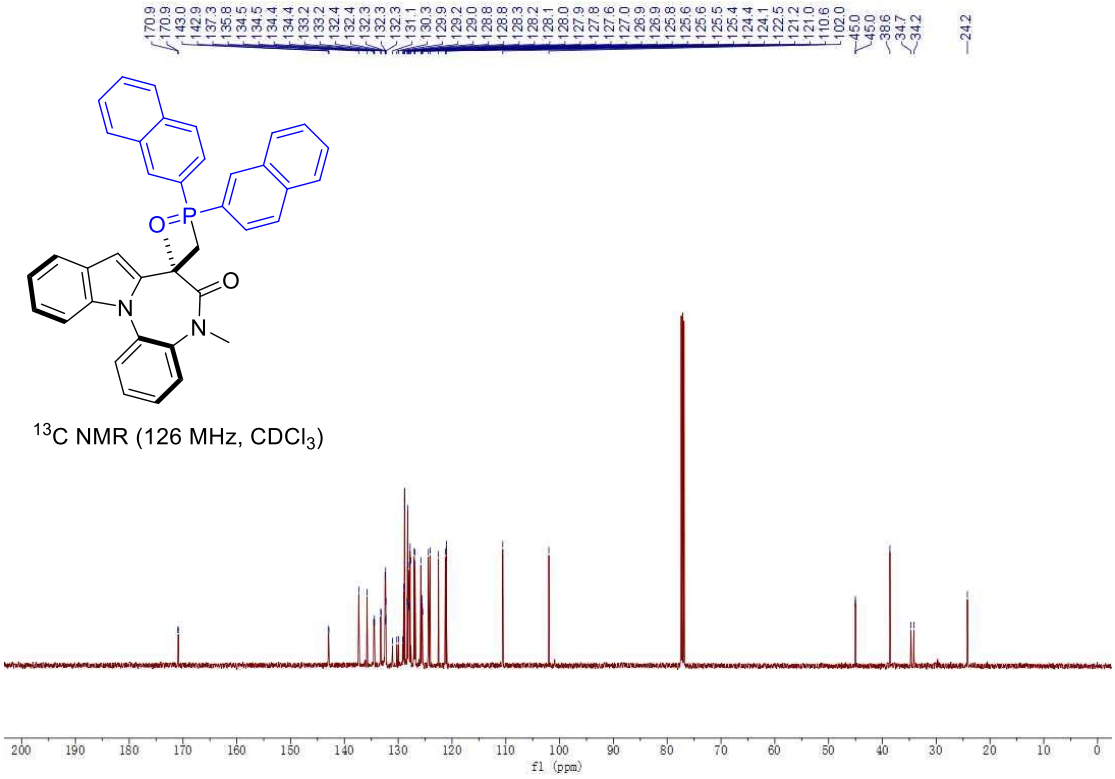
7-((di(naphthalen-2-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3s)



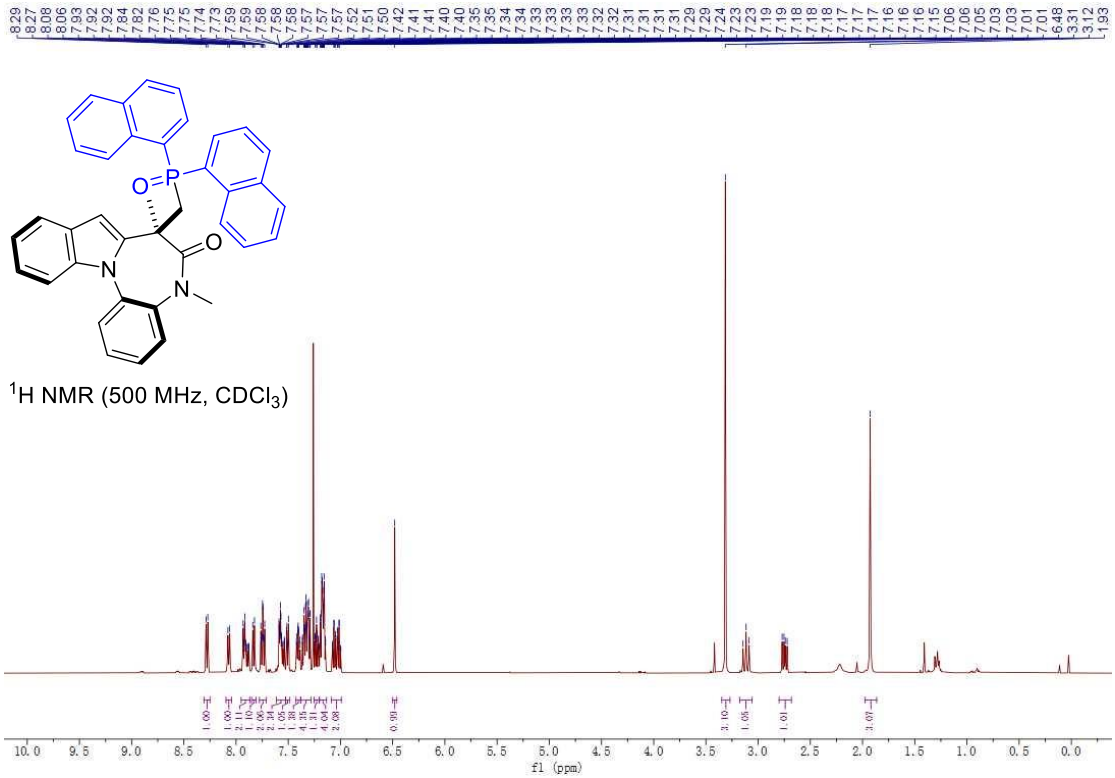
7-((di(naphthalen-2-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3s)



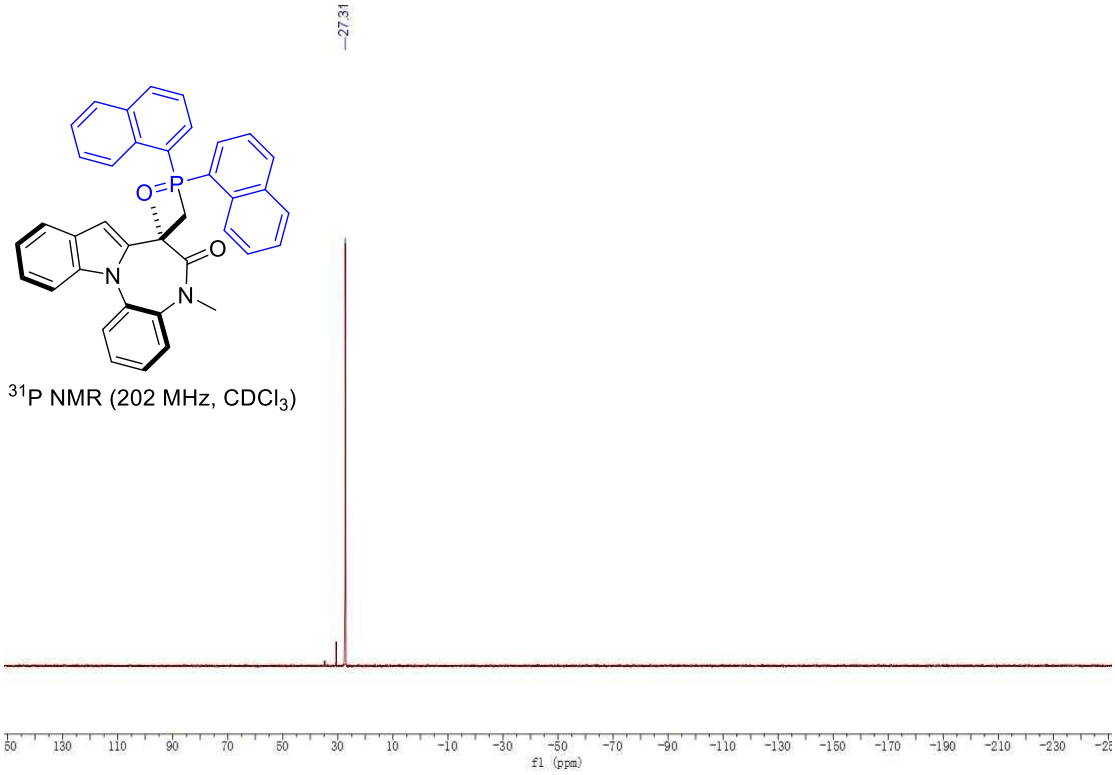
7-((di(naphthalen-2-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3s)



7-((di(naphthalen-1-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3t)

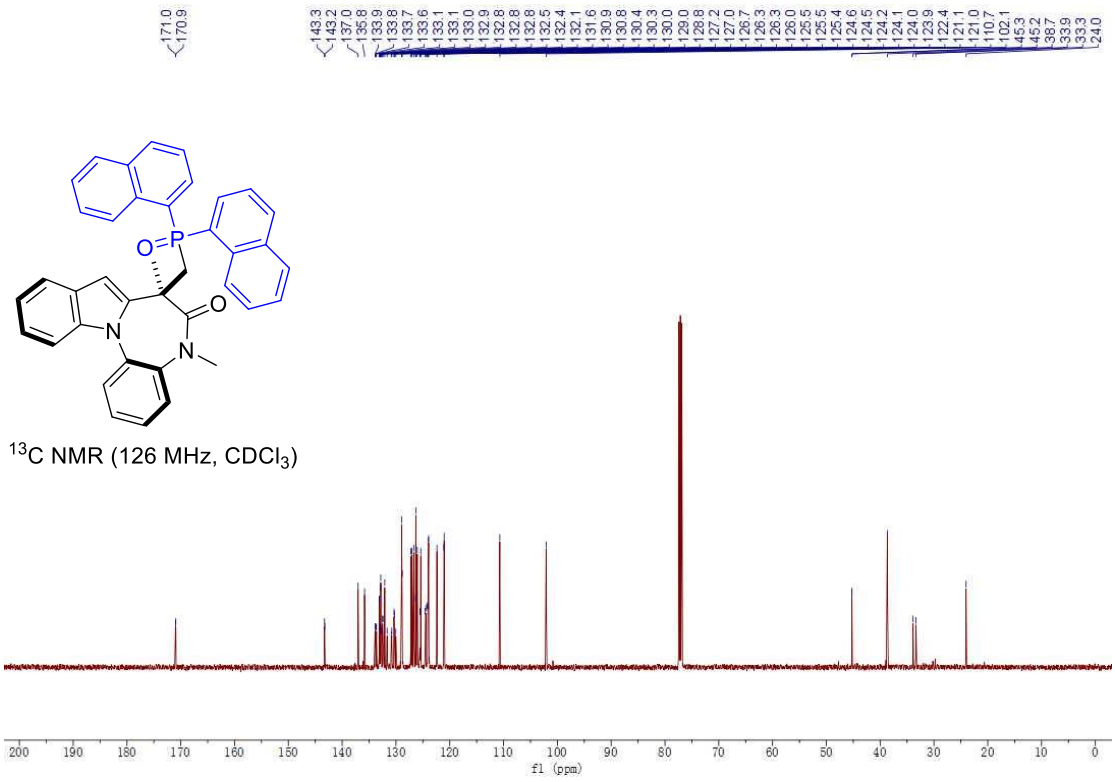


7-((di(naphthalen-1-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3t)



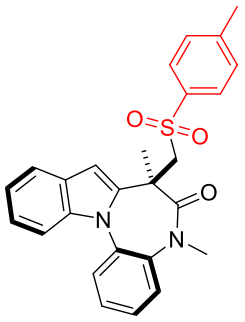
^{31}P NMR (202 MHz, $CDCl_3$)

7-((di(naphthalen-1-yl)phosphoryl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (3t)

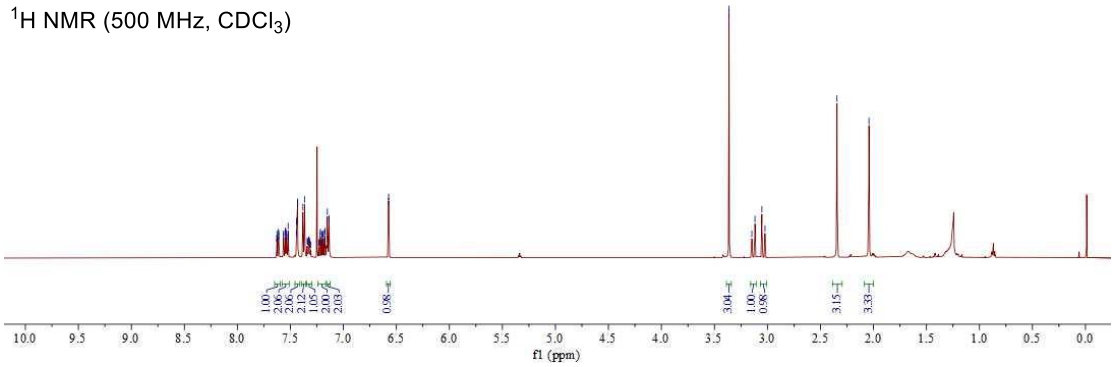


^{13}C NMR (126 MHz, $CDCl_3$)

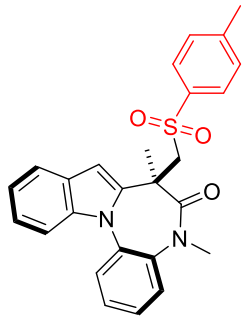
5,7-dimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5a)



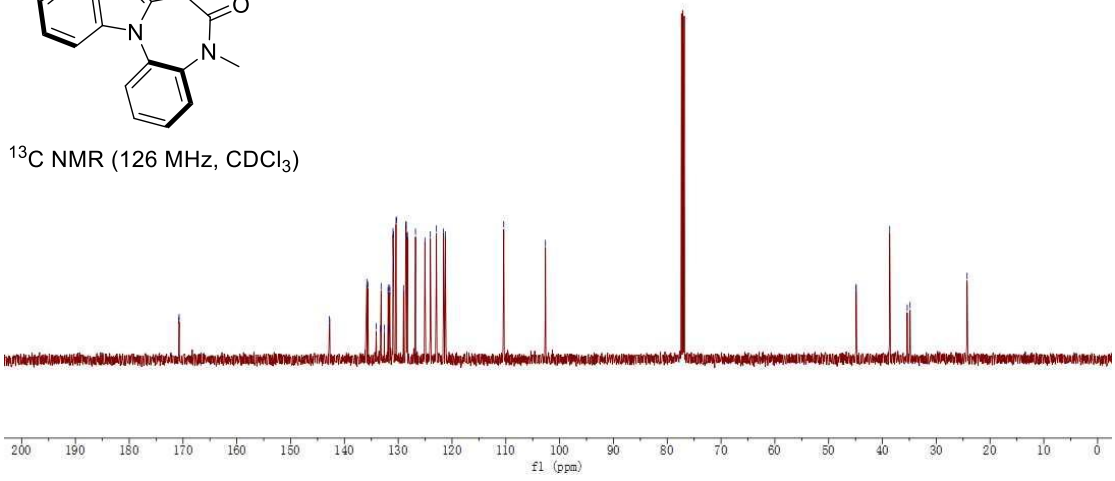
^{1}H NMR (500 MHz, $CDCl_3$)



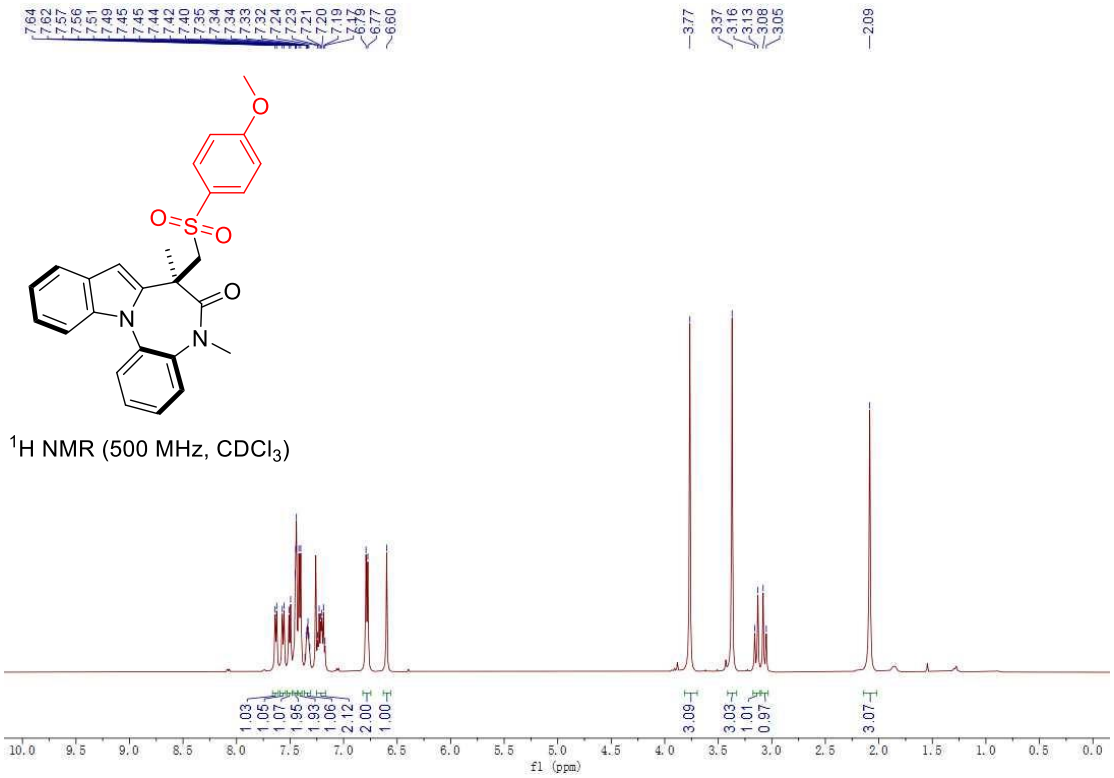
5,7-dimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5a)



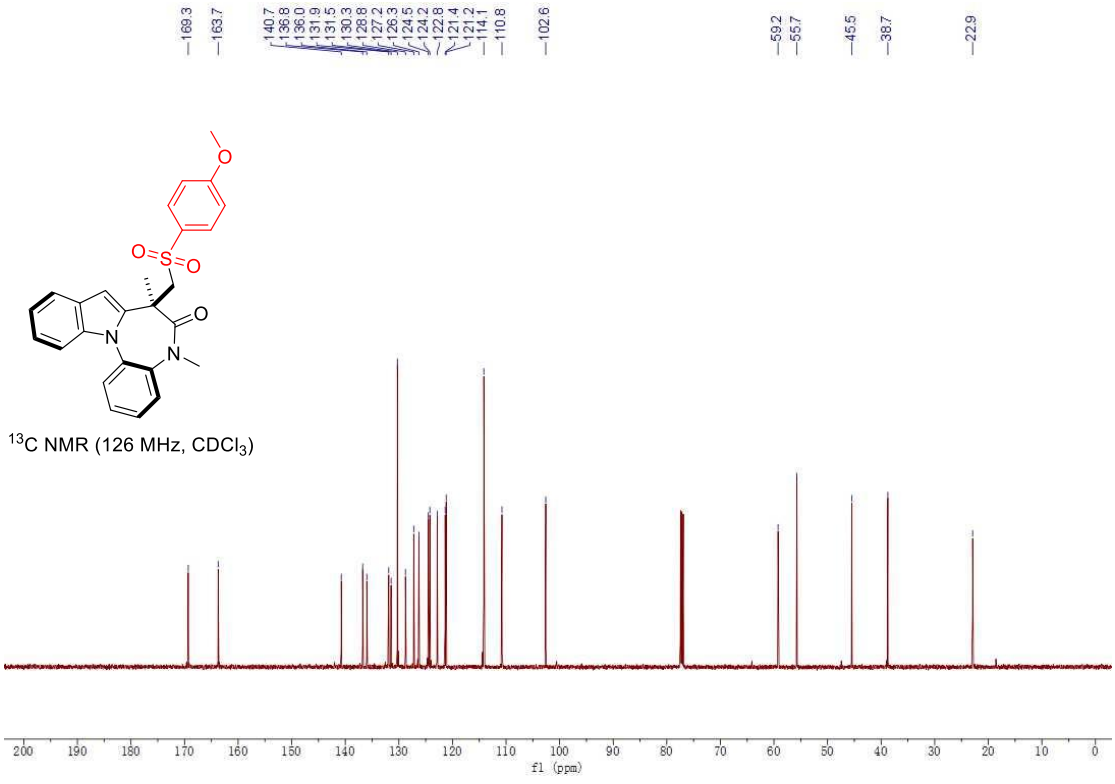
^{13}C NMR (126 MHz, $CDCl_3$)



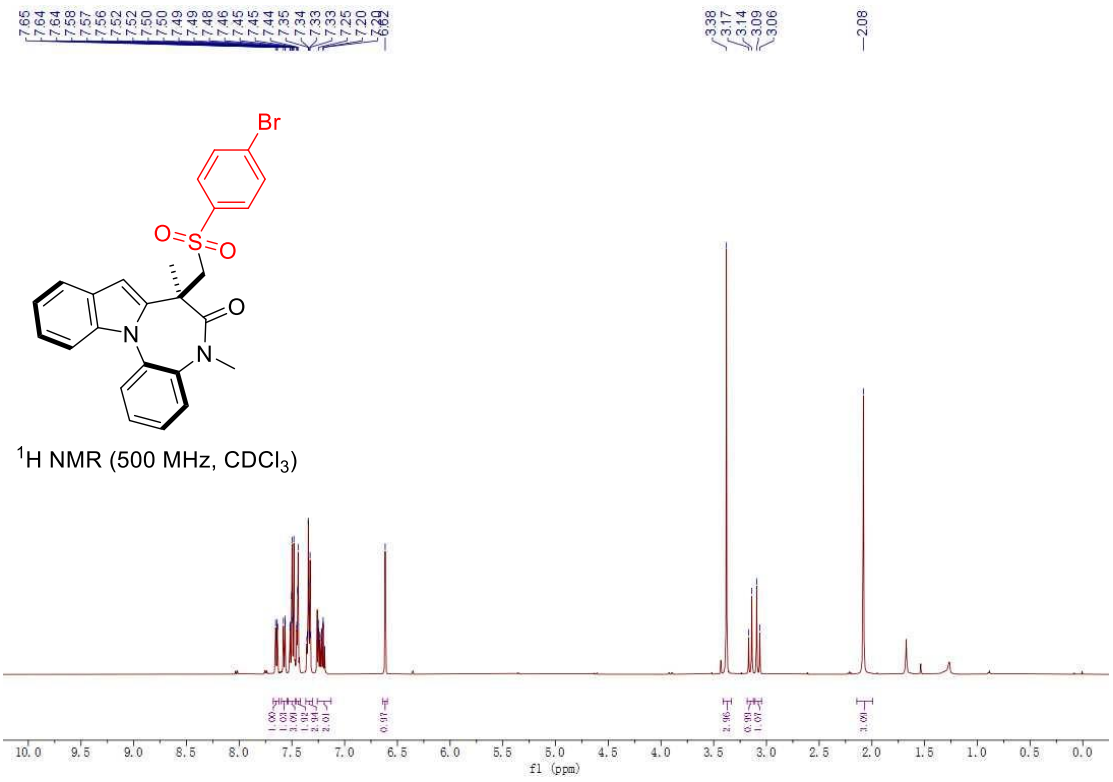
7-(((4-methoxyphenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5b)



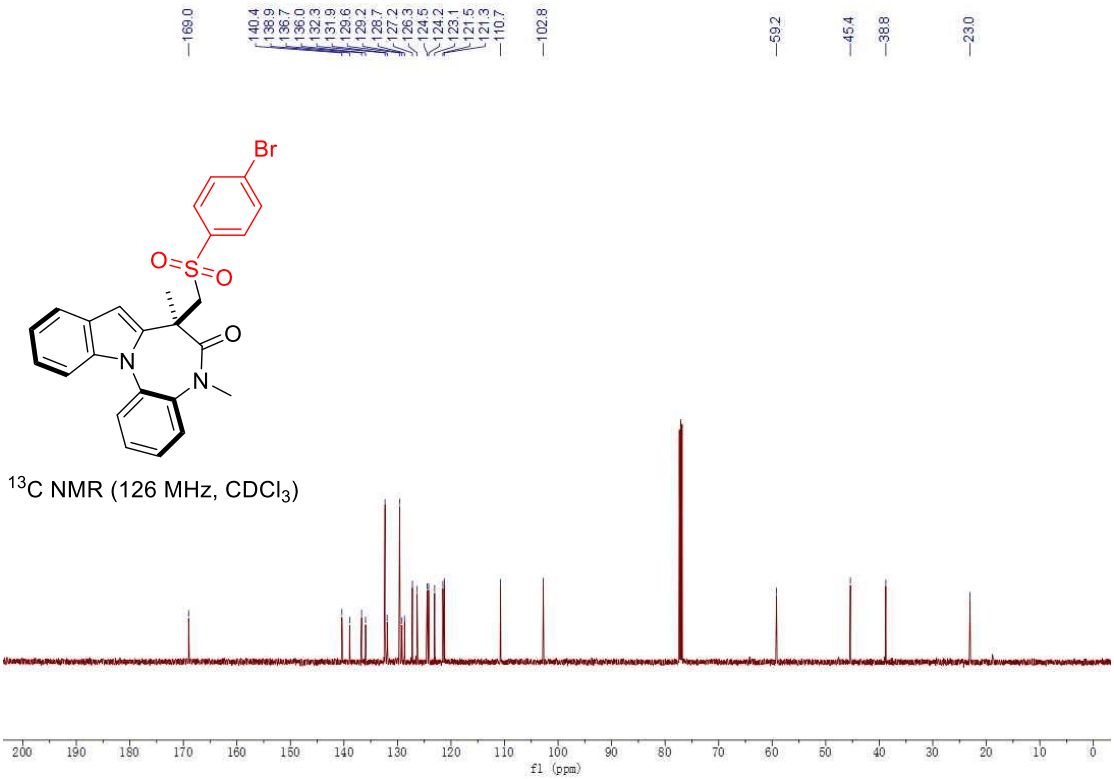
7-(((4-methoxyphenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5b)



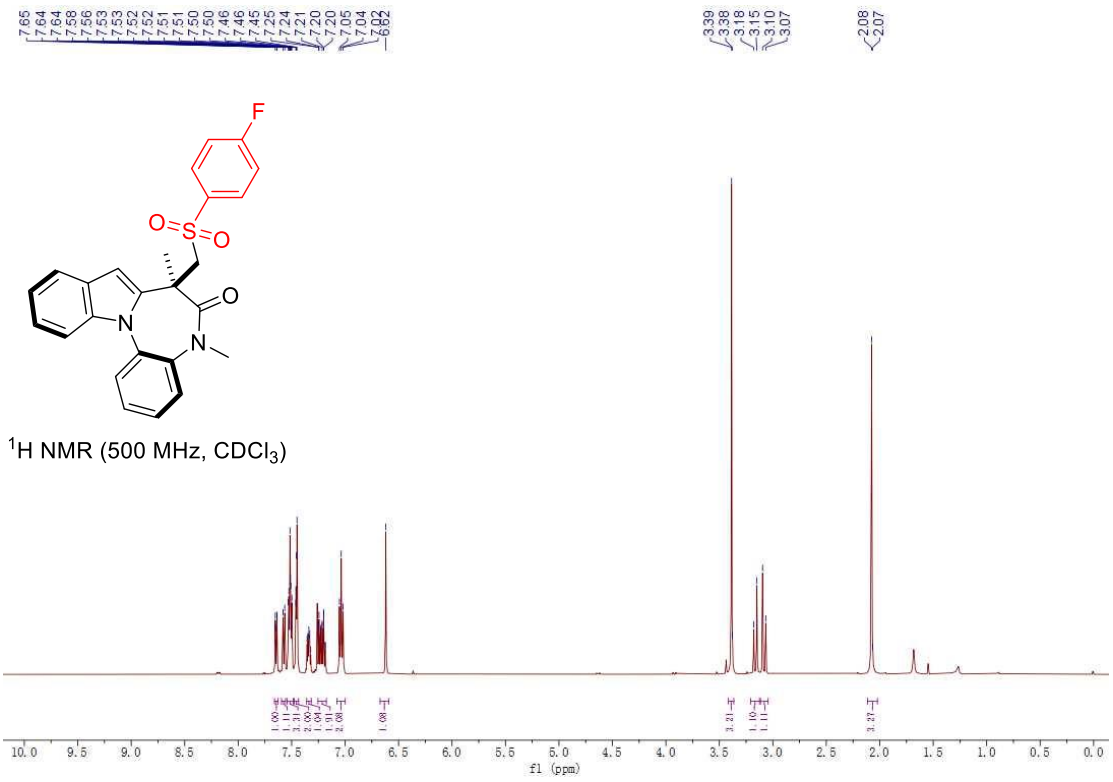
7-(((4-bromophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5c)



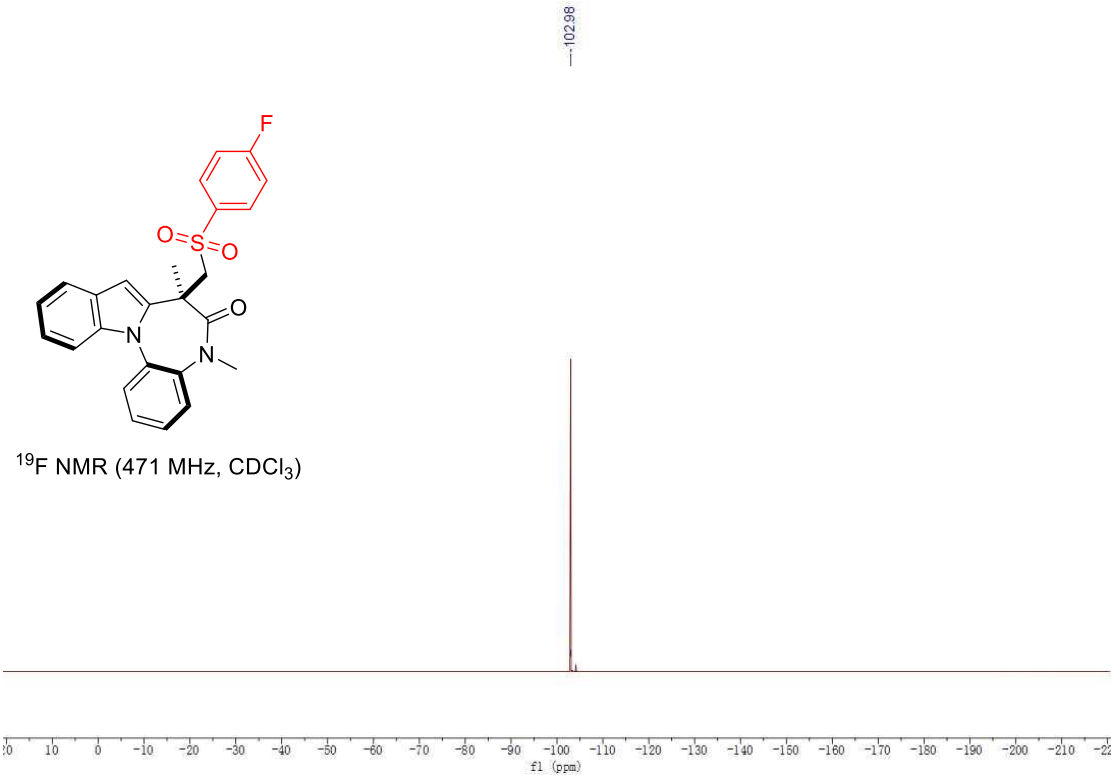
7-(((4-bromophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5c)



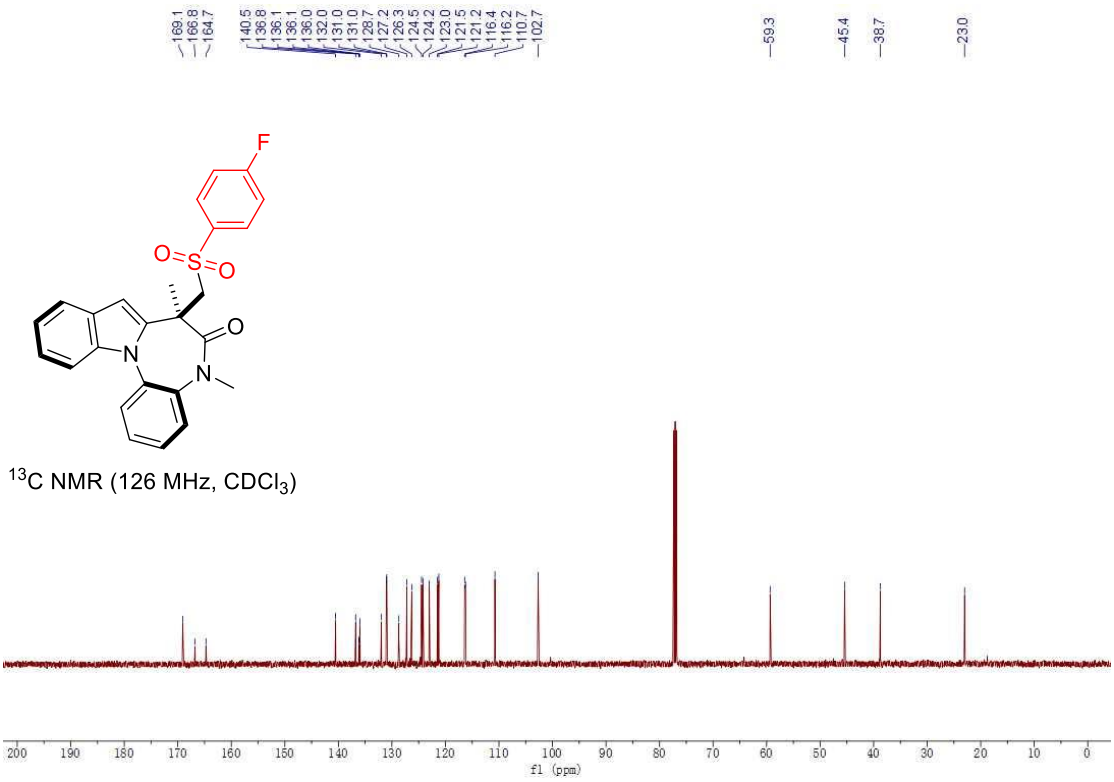
7-(((4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5d)



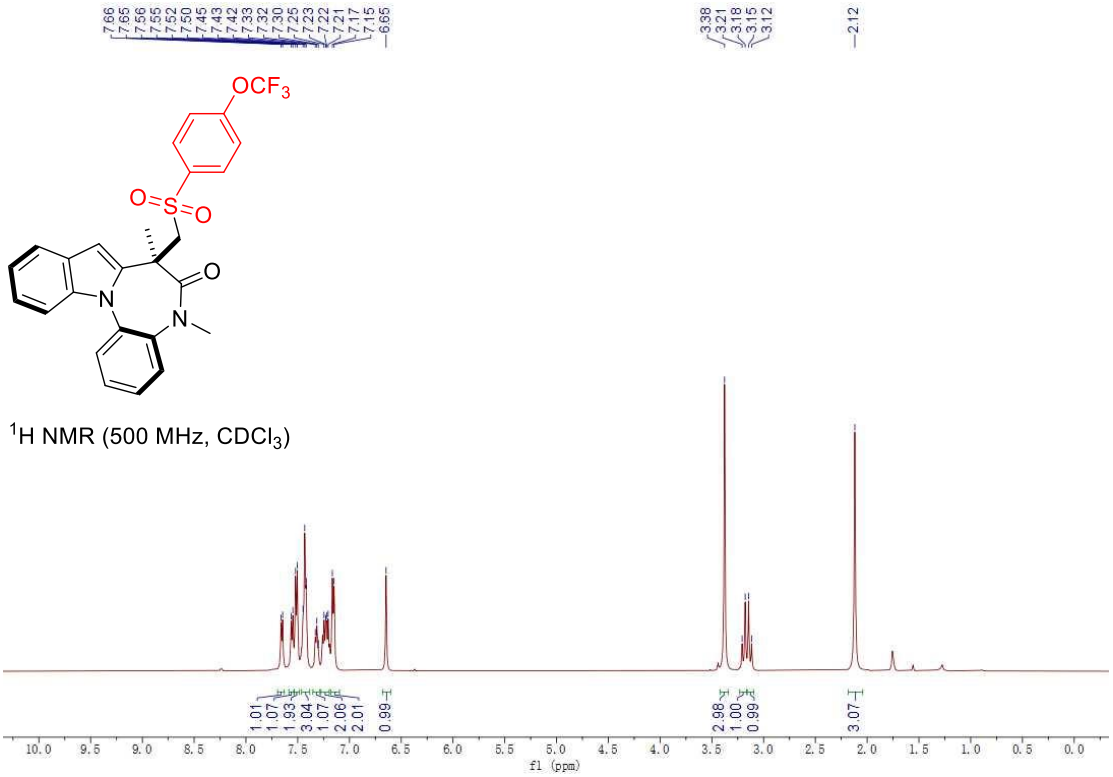
7-(((4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5d)



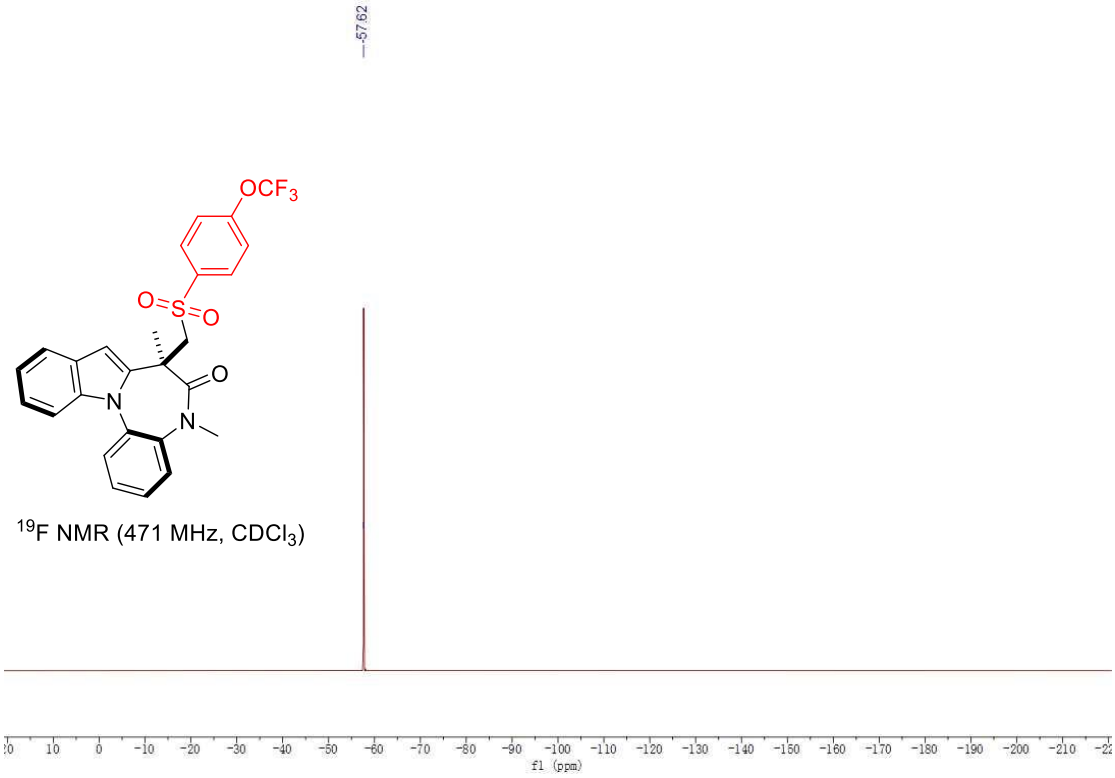
7-(((4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5d)



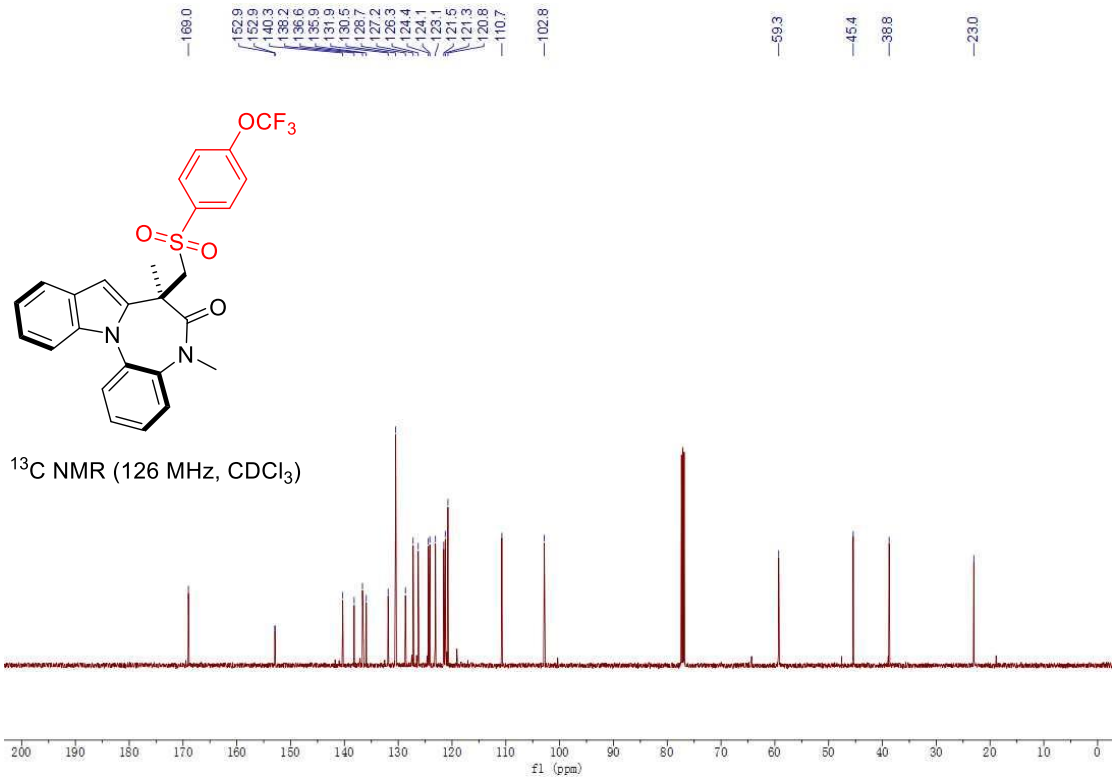
5,7-dimethyl-7-(((4-(trifluoromethoxy)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5e)



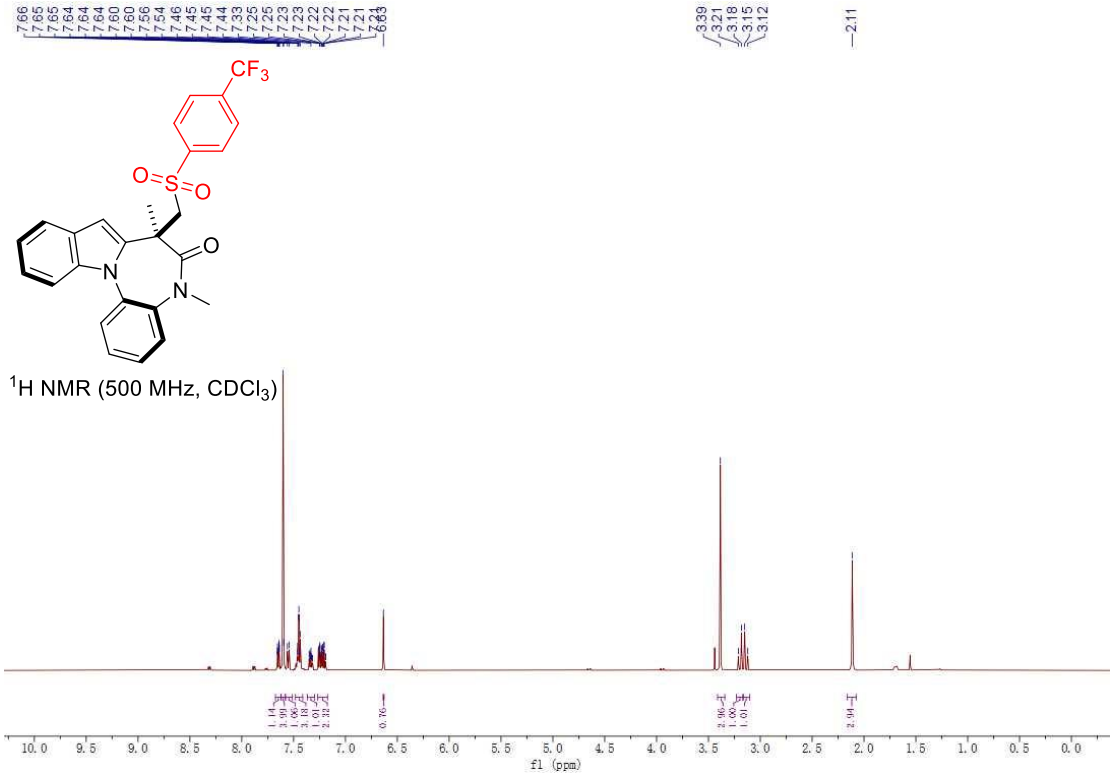
5,7-dimethyl-7-(((4-(trifluoromethoxy)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5e)



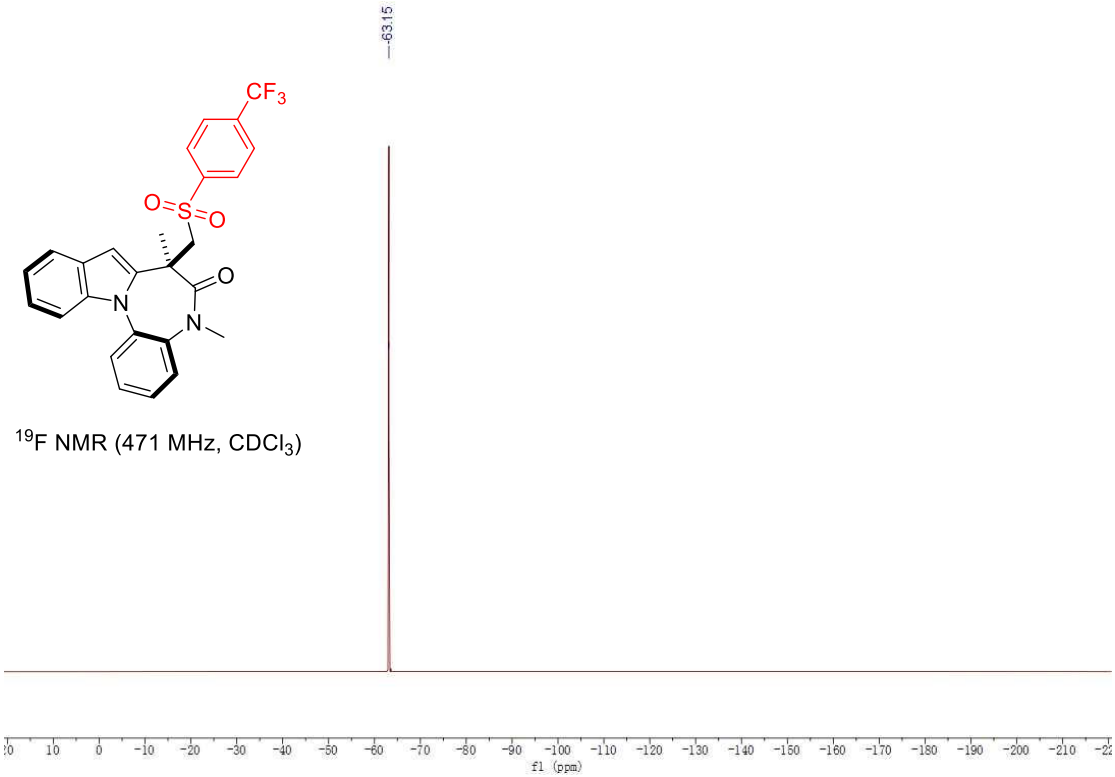
5,7-dimethyl-7-(((4-(trifluoromethoxy)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5e)



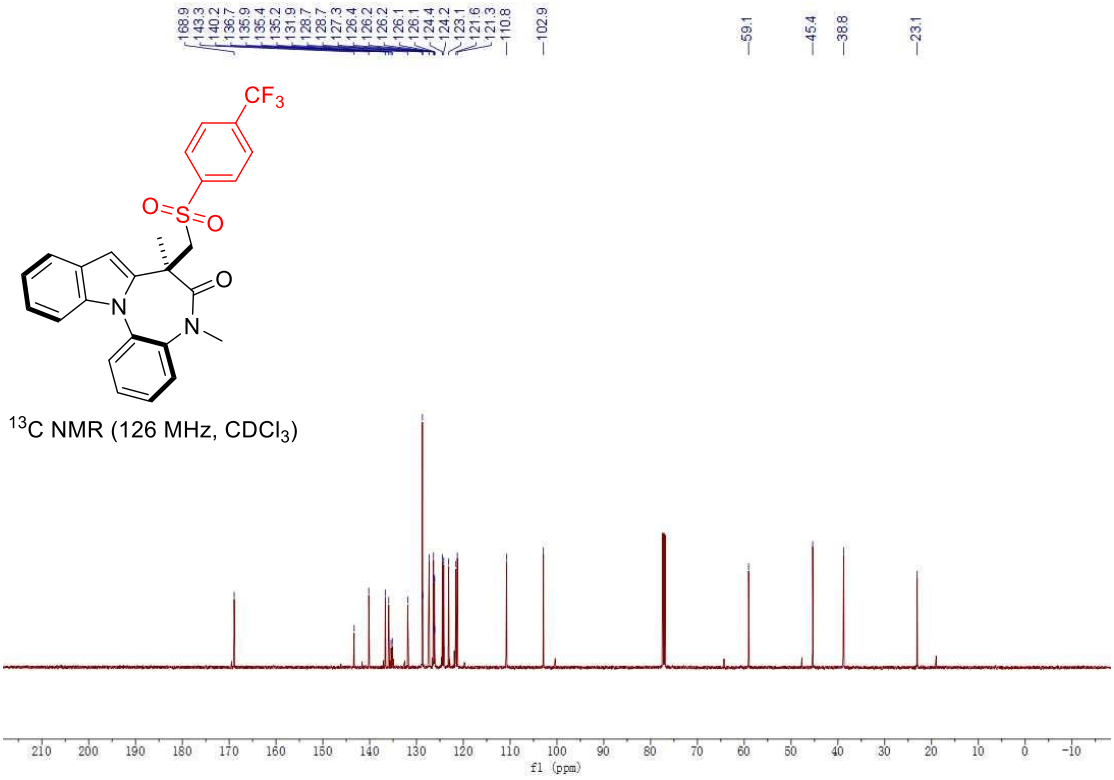
5,7-dimethyl-7-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5f)



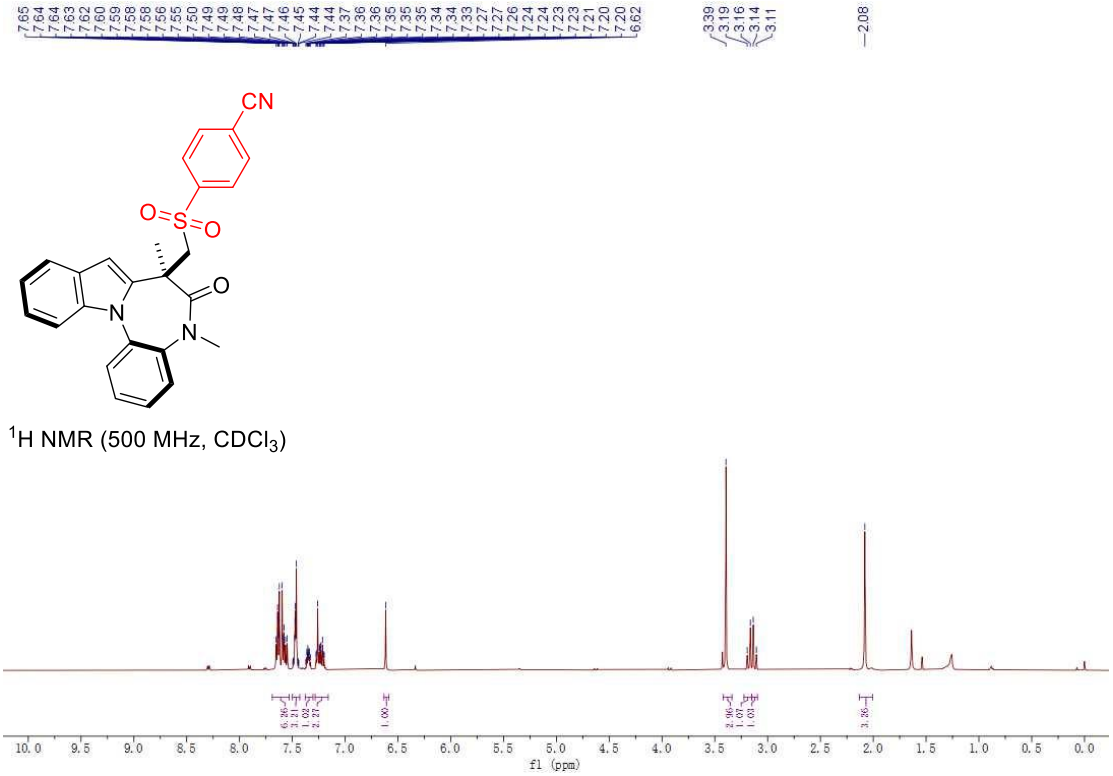
5,7-dimethyl-7-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5f)



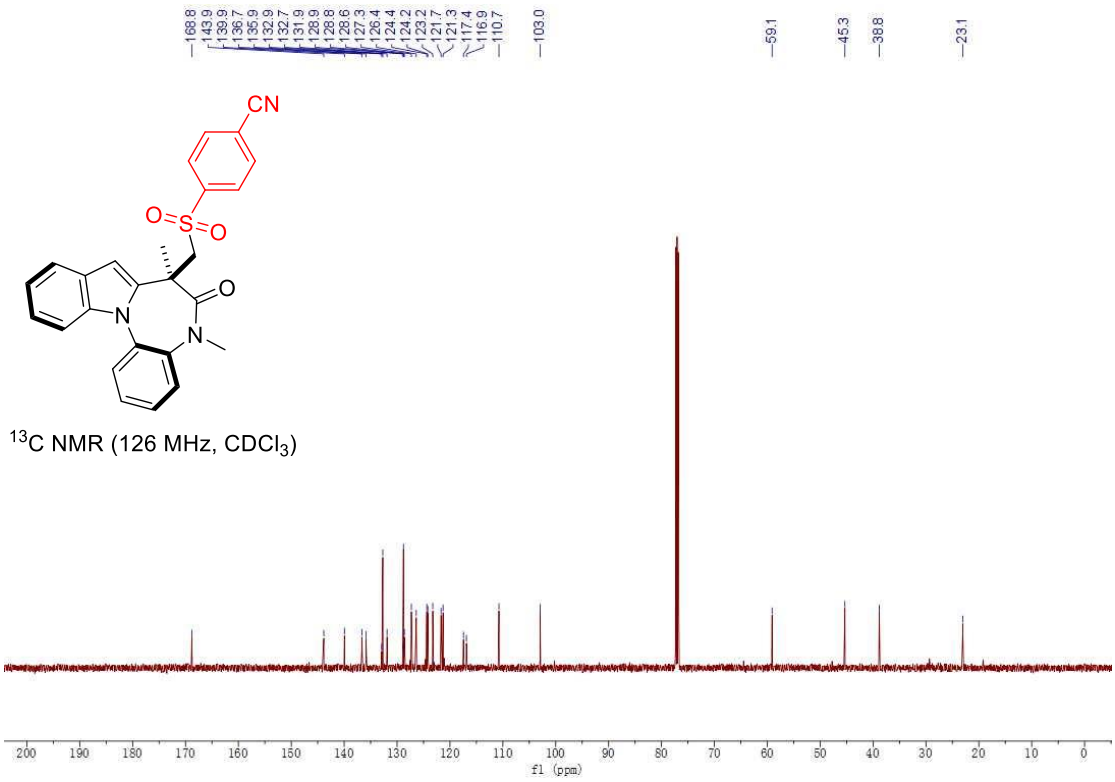
5,7-dimethyl-7-(((4-(trifluoromethyl)phenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5f)



4-(((5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-7-yl)methyl)sulfonyl)benzonitrile (5g)

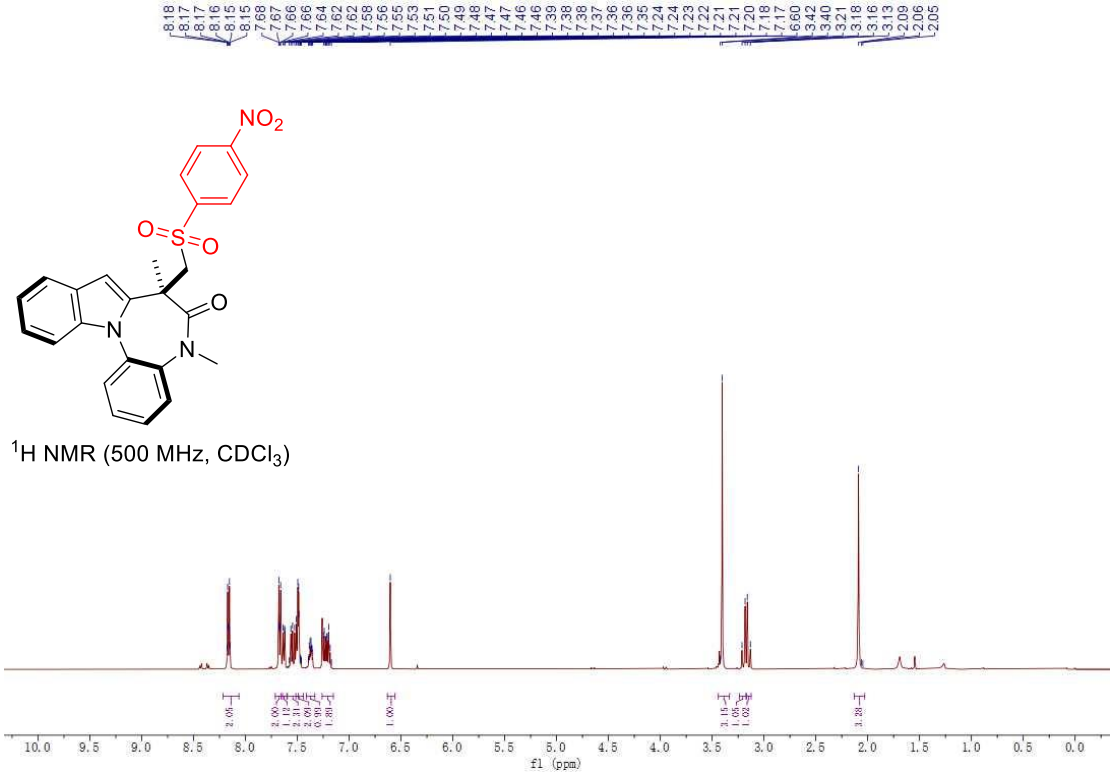


4-(((5,7-dimethyl-6-oxo-6,7-dihydro-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-7-yl)methyl)sulfonyl)benzonitrile (5g)



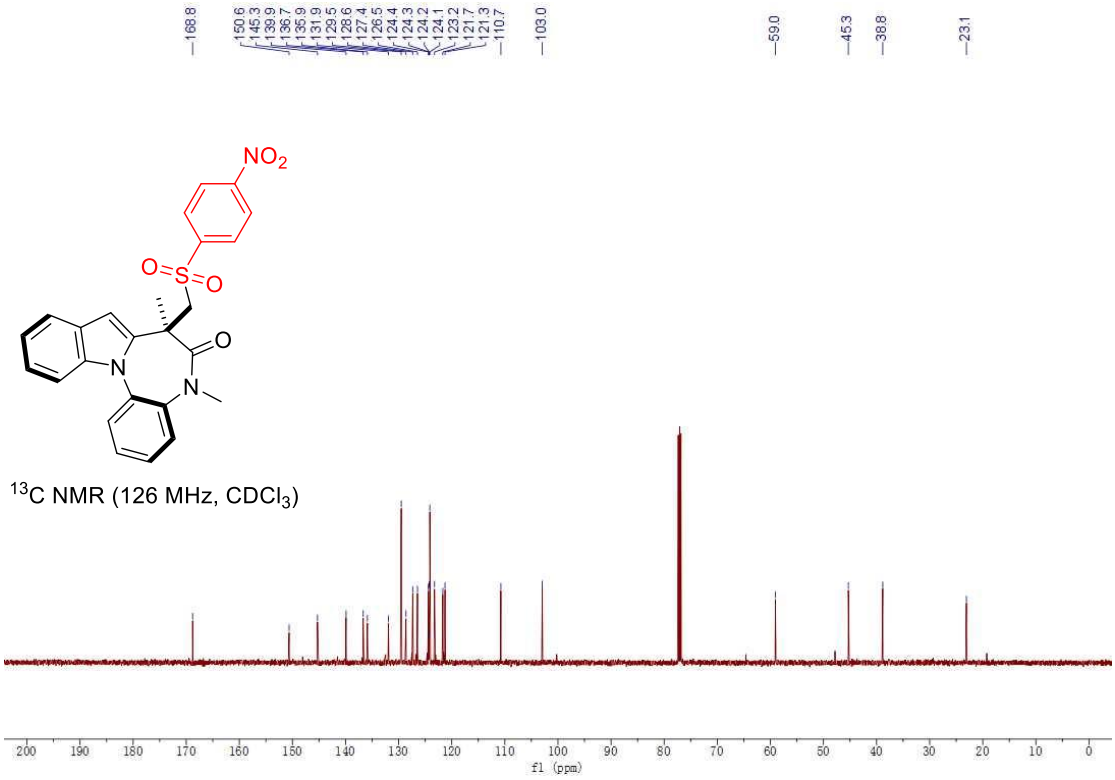
^{13}C NMR (126 MHz, $CDCl_3$)

5,7-dimethyl-7-(((4-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5h)

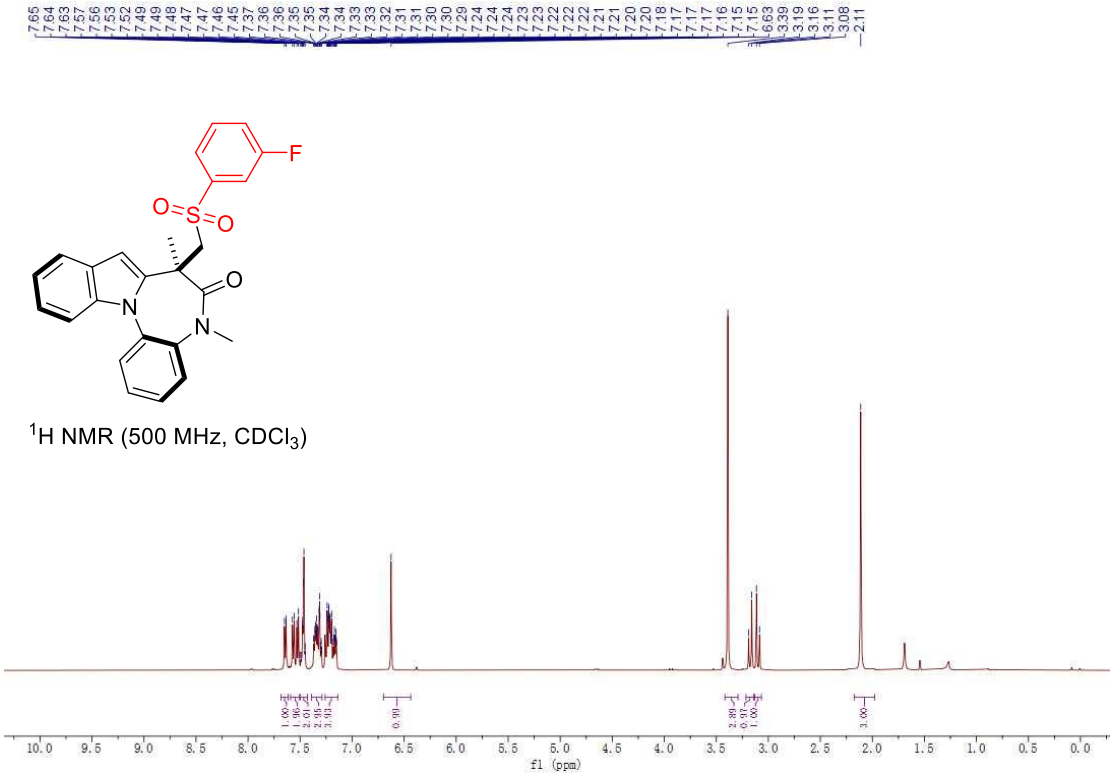


^{1}H NMR (500 MHz, $CDCl_3$)

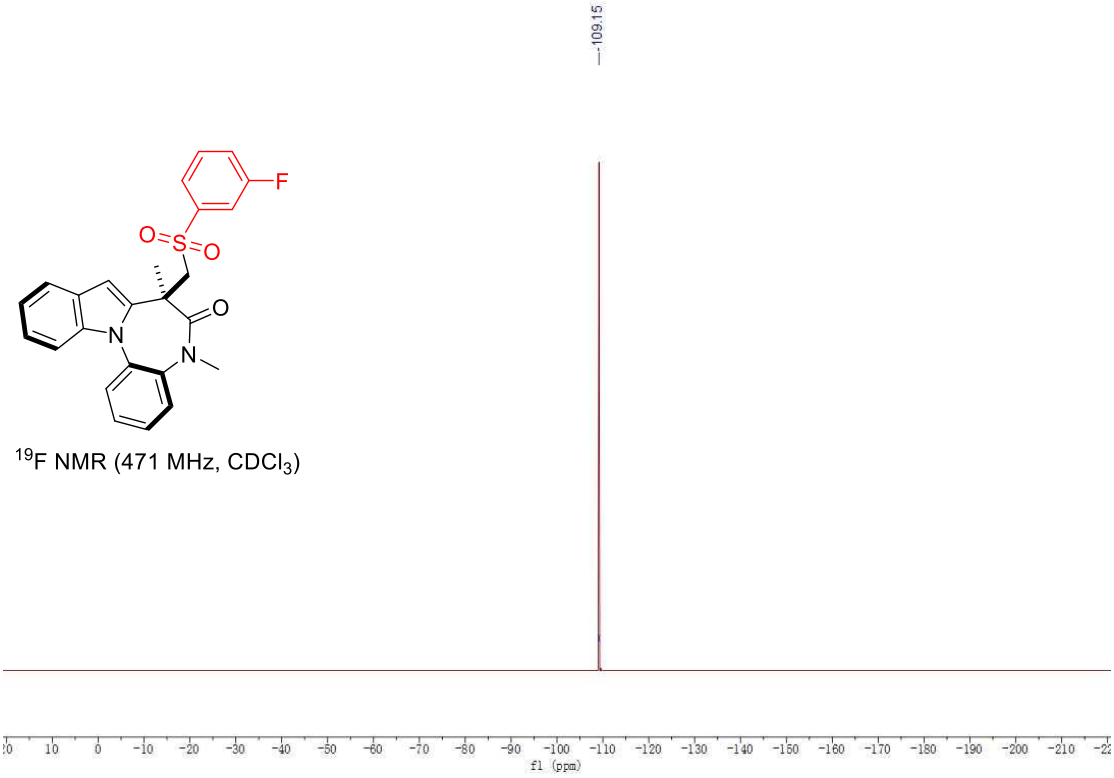
5,7-dimethyl-7-(((4-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5h)



7-(((3-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5i)

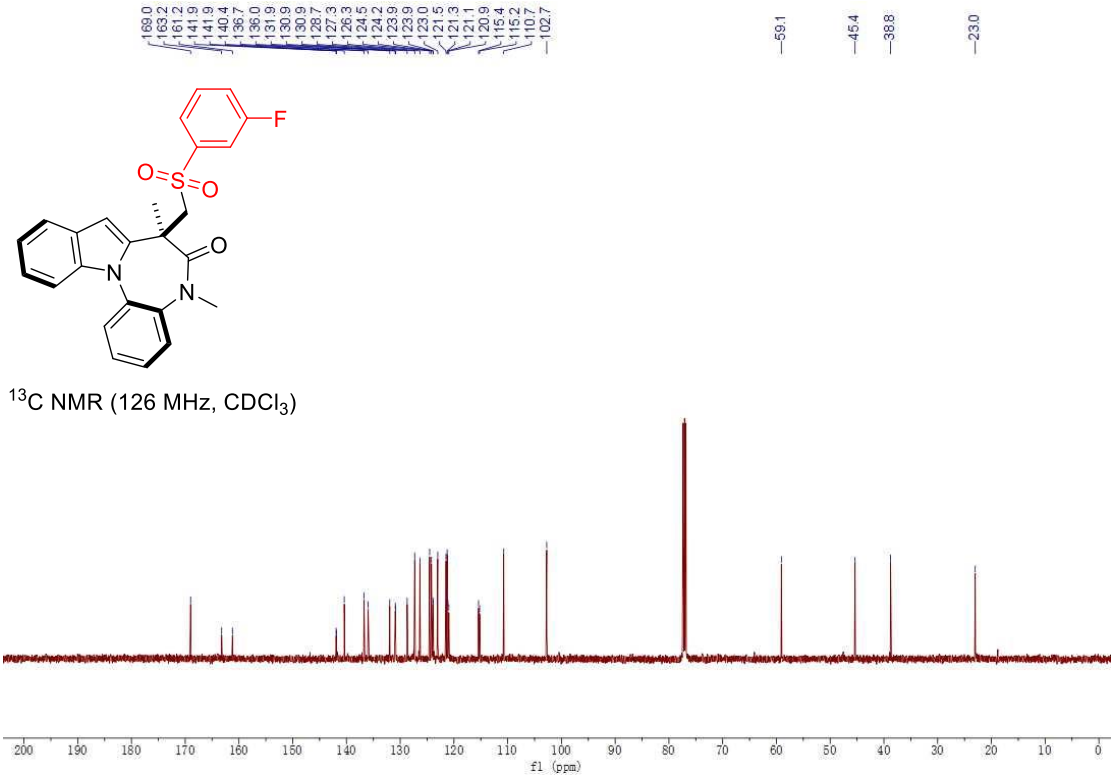


7-(((3-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5i)



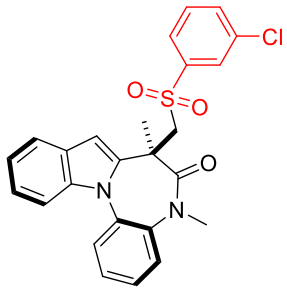
^{19}F NMR (471 MHz, $CDCl_3$)

7-(((3-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5i)

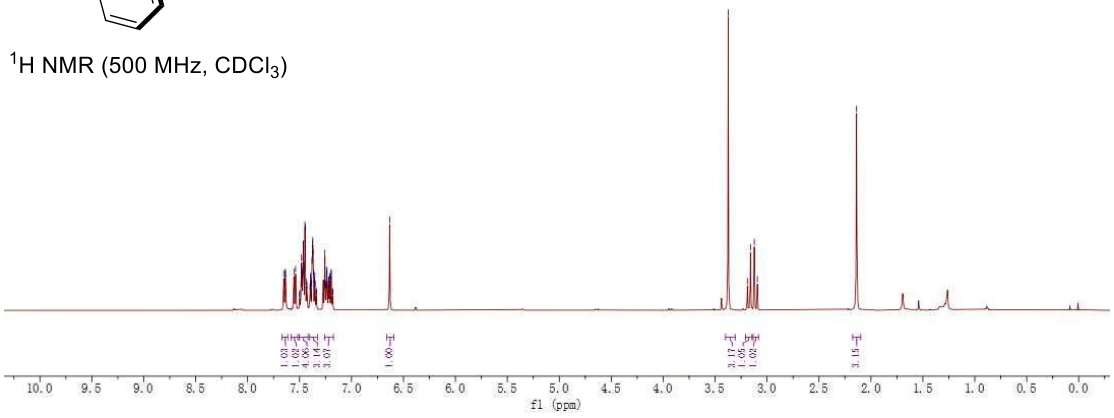


^{13}C NMR (126 MHz, $CDCl_3$)

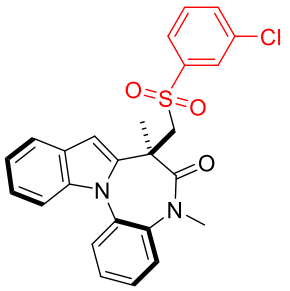
7-(((3-chlorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5j)



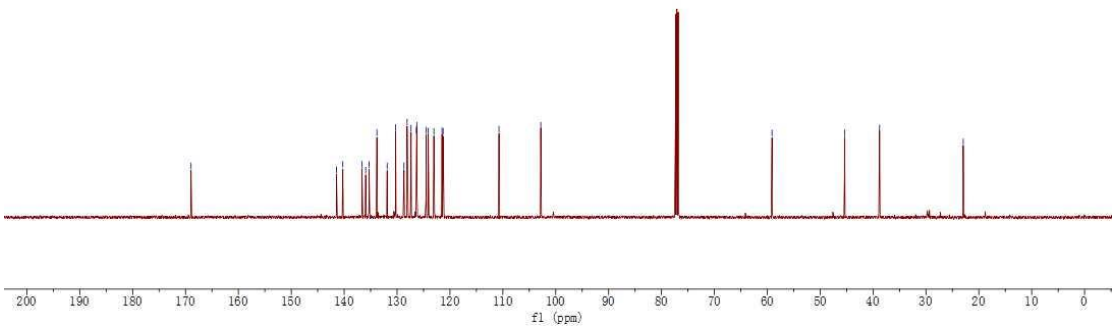
^{1}H NMR (500 MHz, $CDCl_3$)



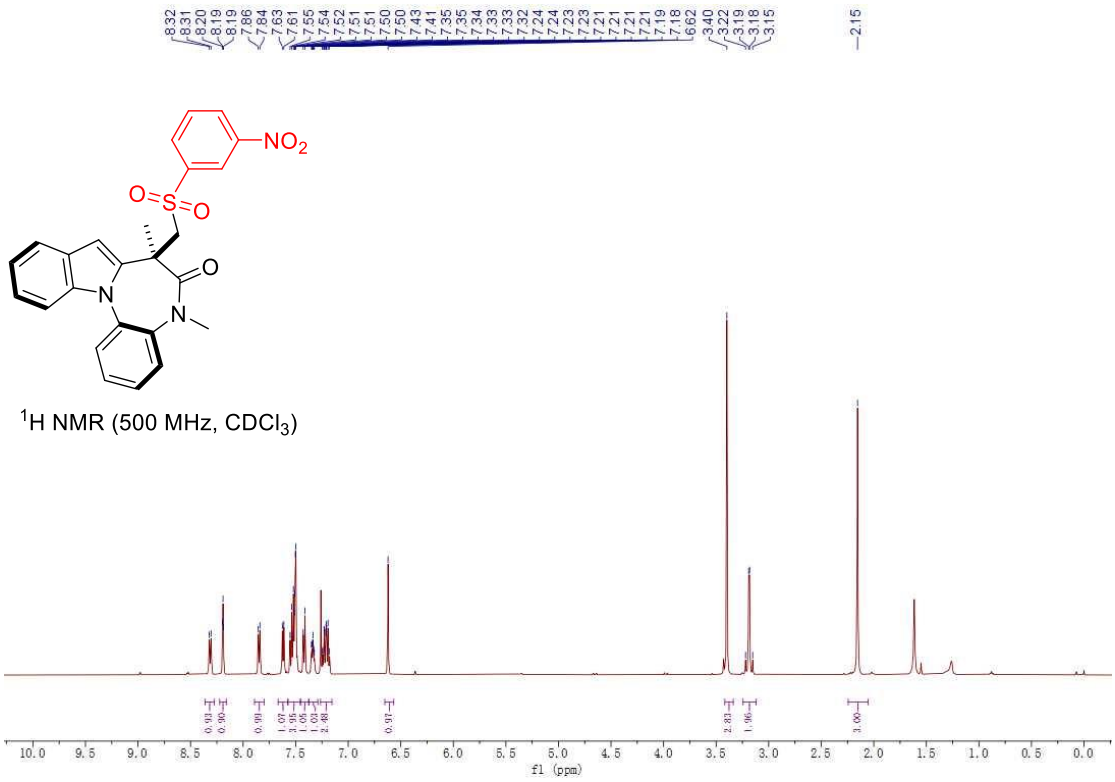
7-(((3-chlorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5j)



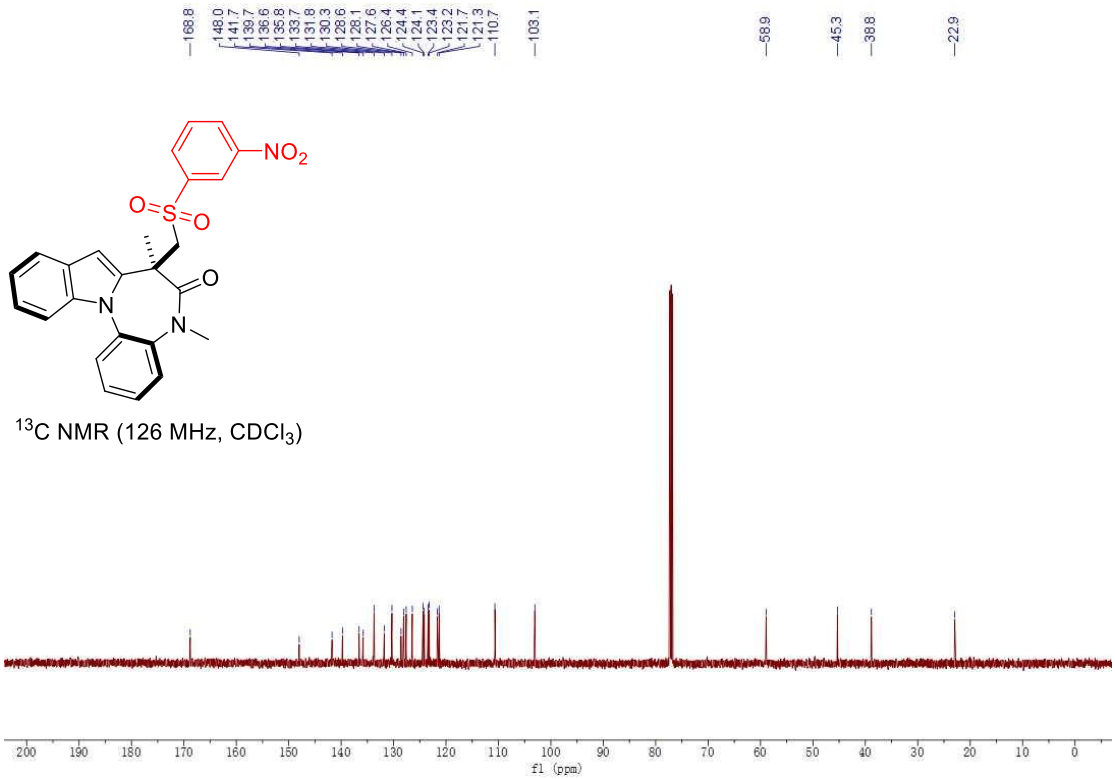
^{13}C NMR (126 MHz, $CDCl_3$)



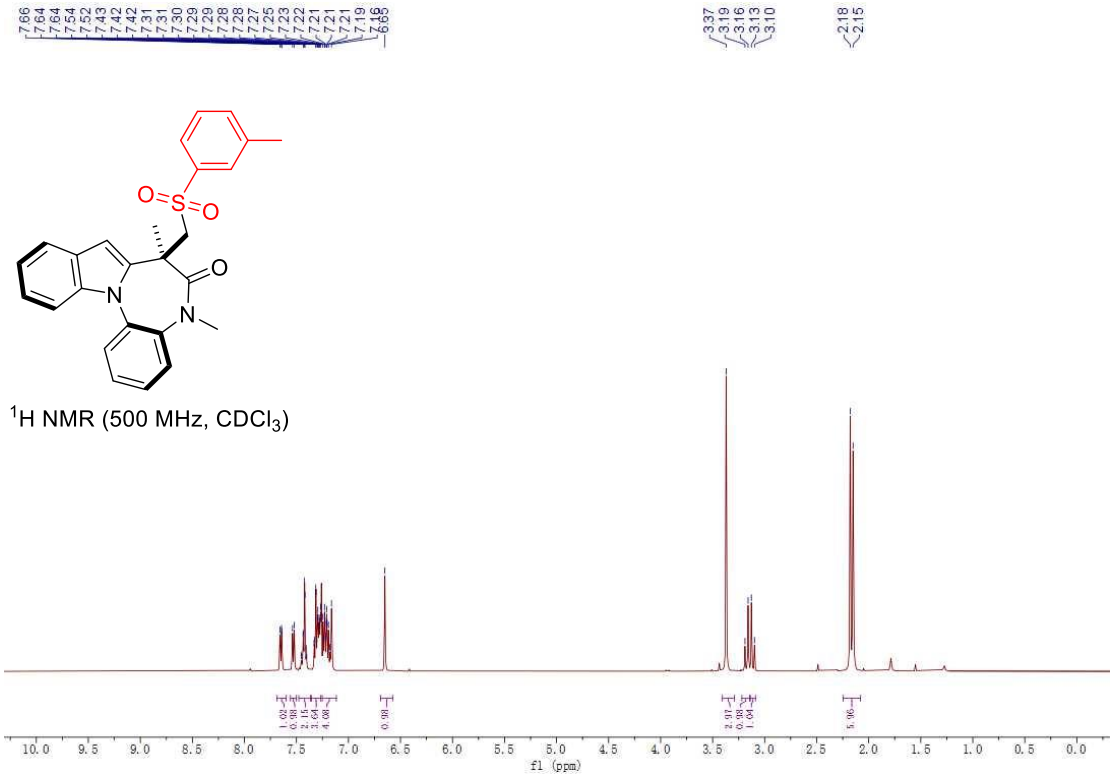
5,7-dimethyl-7-(((3-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5k)



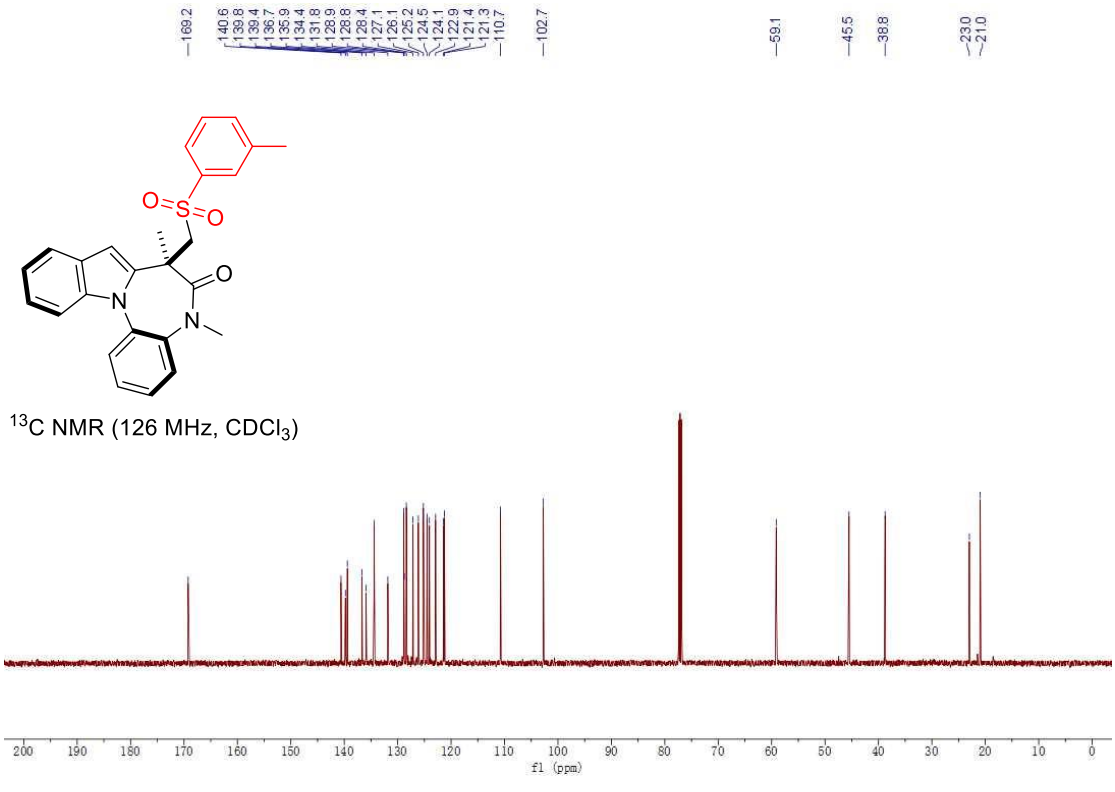
5,7-dimethyl-7-(((3-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one（5k）



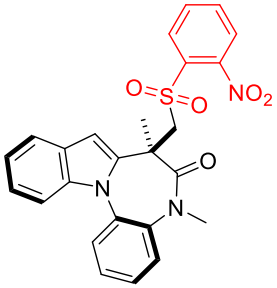
5,7-dimethyl-7-((m-tolylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5l)



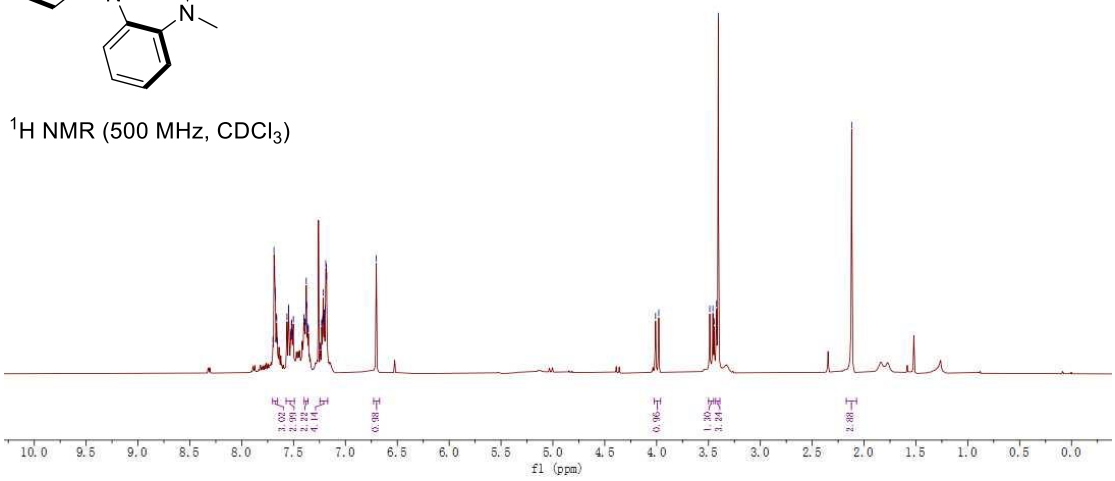
5,7-dimethyl-7-((m-tolylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5l)



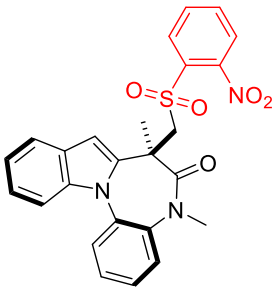
5,7-dimethyl-7-(((2-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5m)



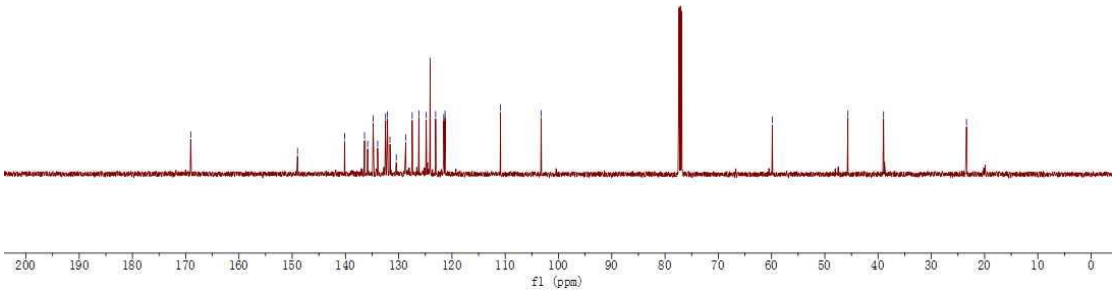
^{1}H NMR (500 MHz, $CDCl_3$)



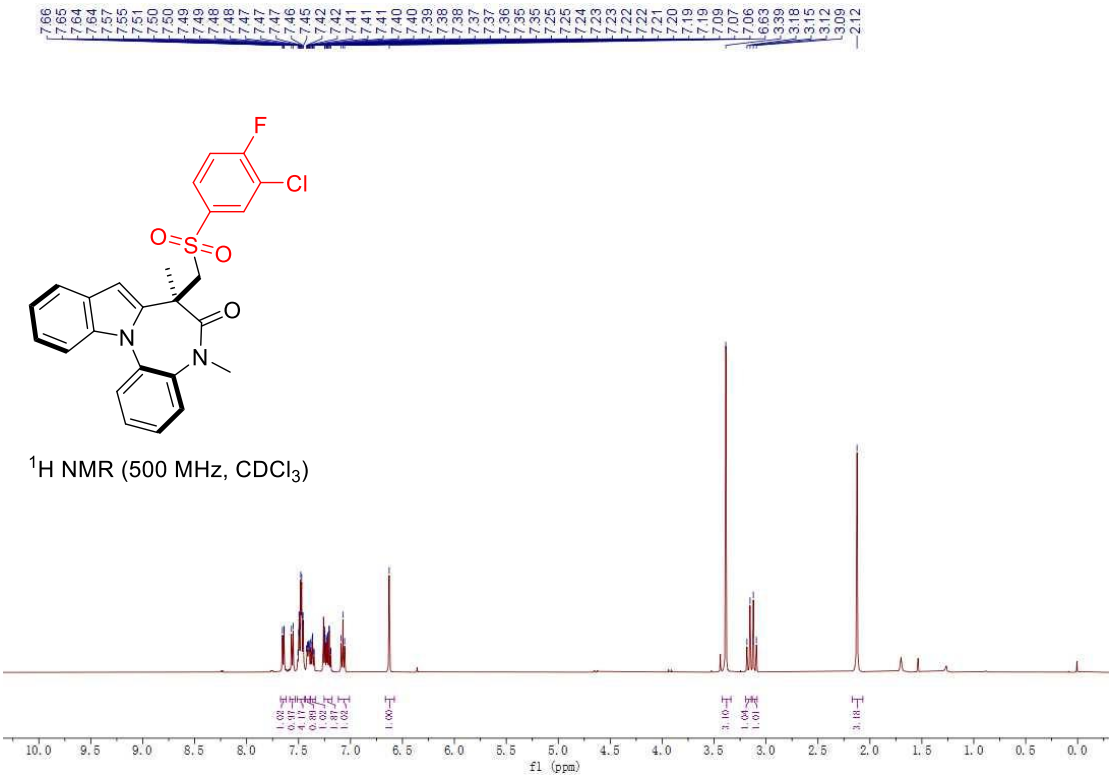
5,7-dimethyl-7-(((2-nitrophenyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5m)



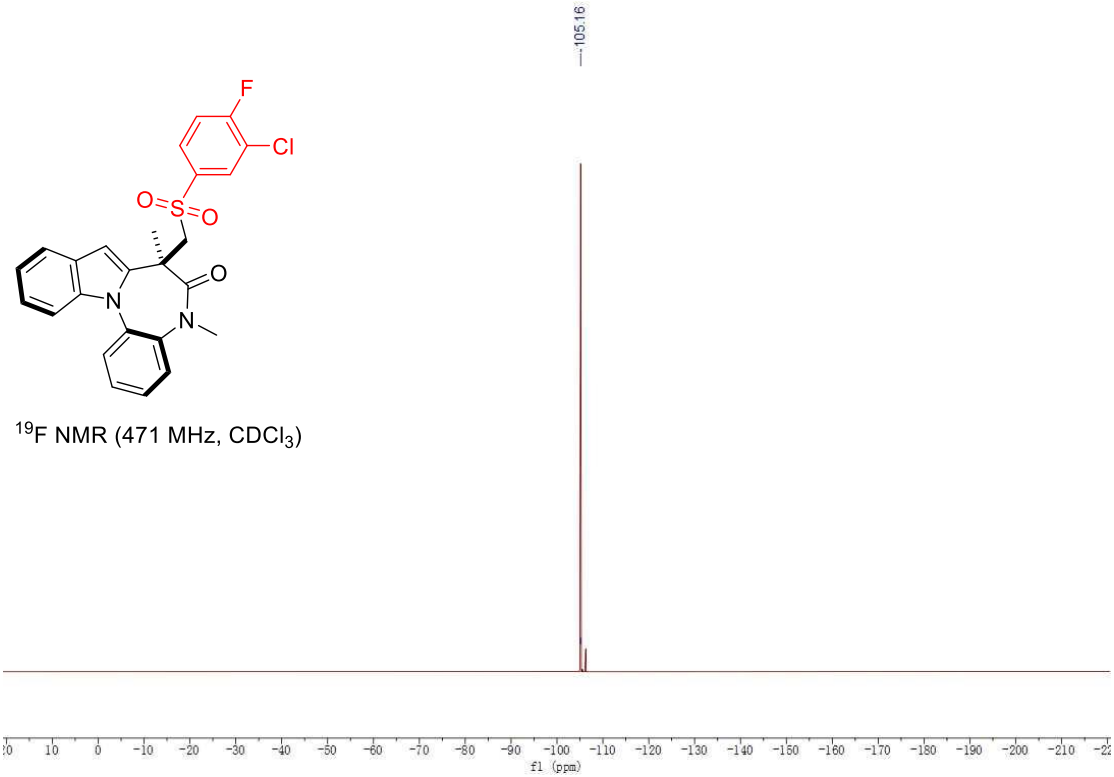
^{13}C NMR (126 MHz, $CDCl_3$)



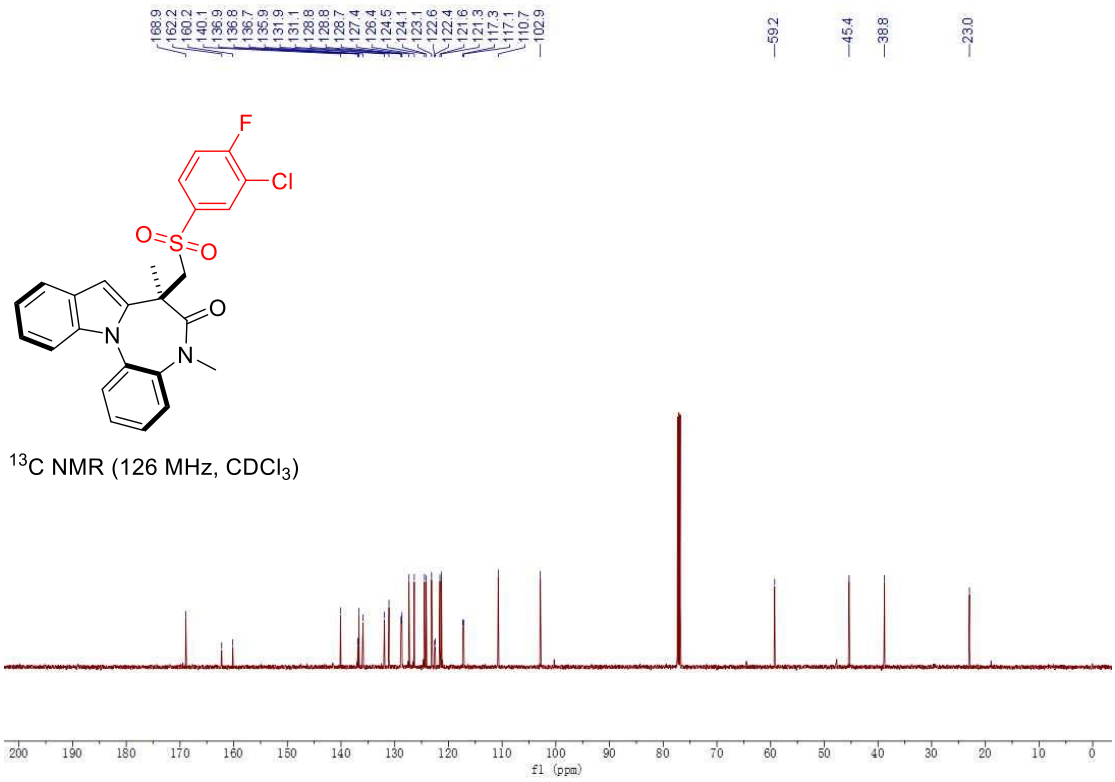
7-(((3-chloro-4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5n)



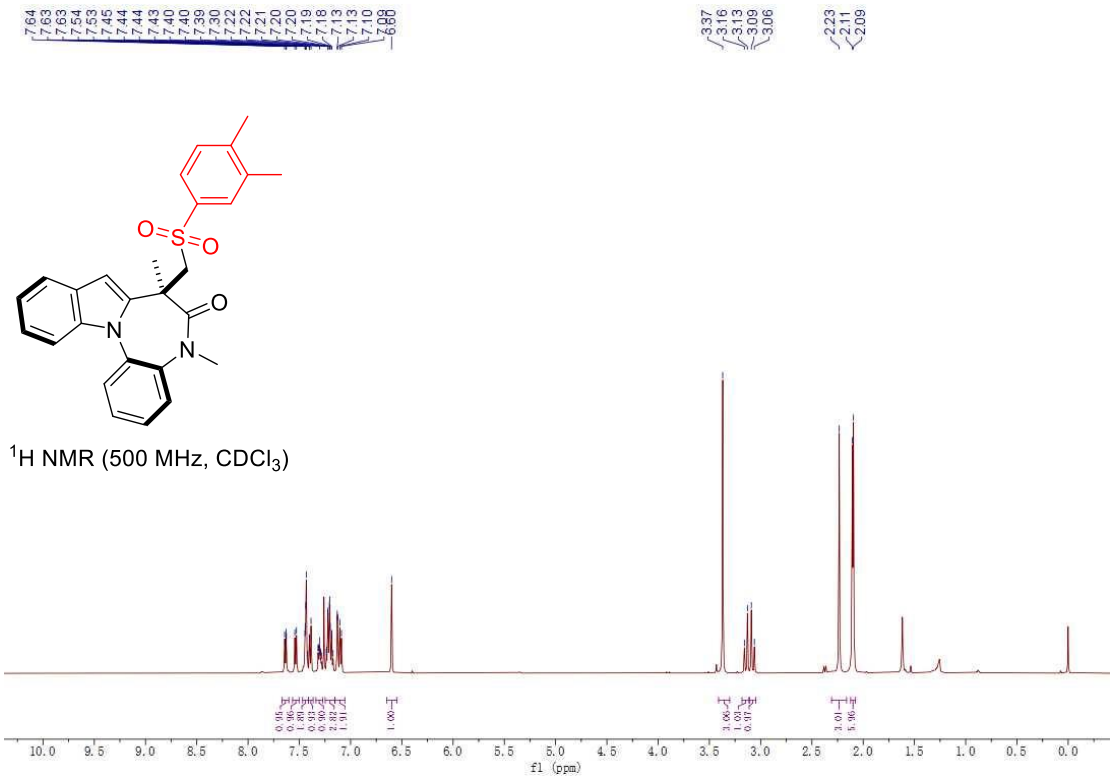
7-(((3-chloro-4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5n)



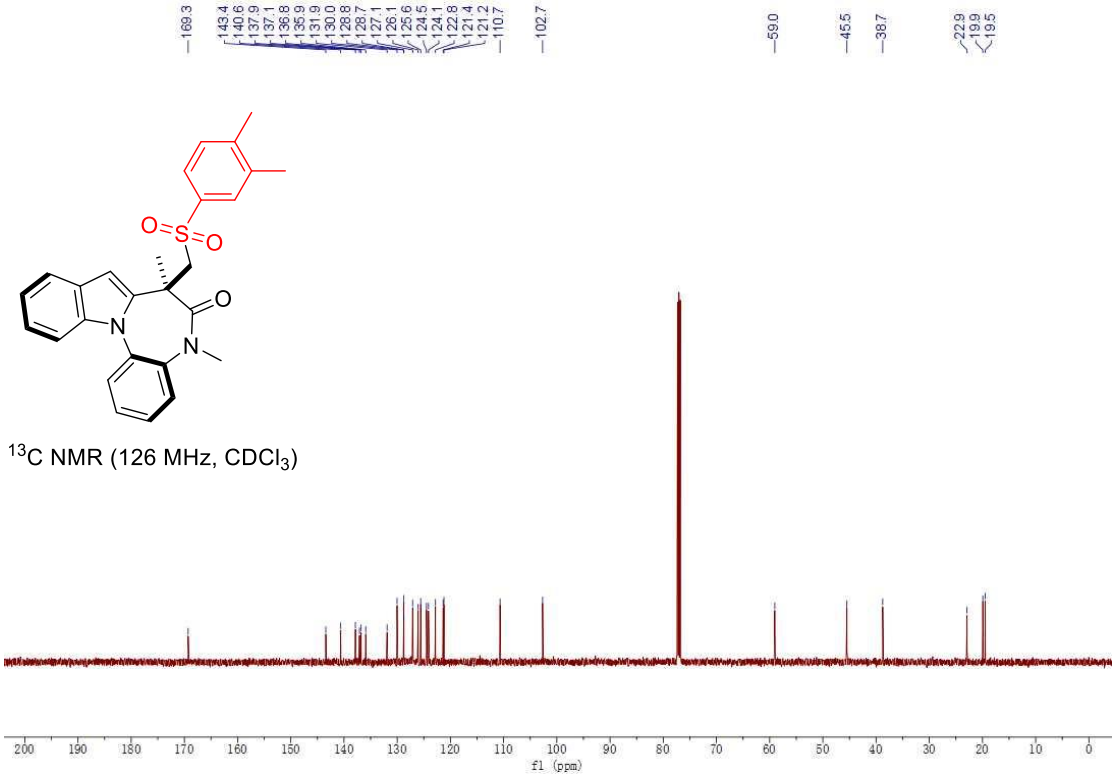
7-(((3-chloro-4-fluorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5n)



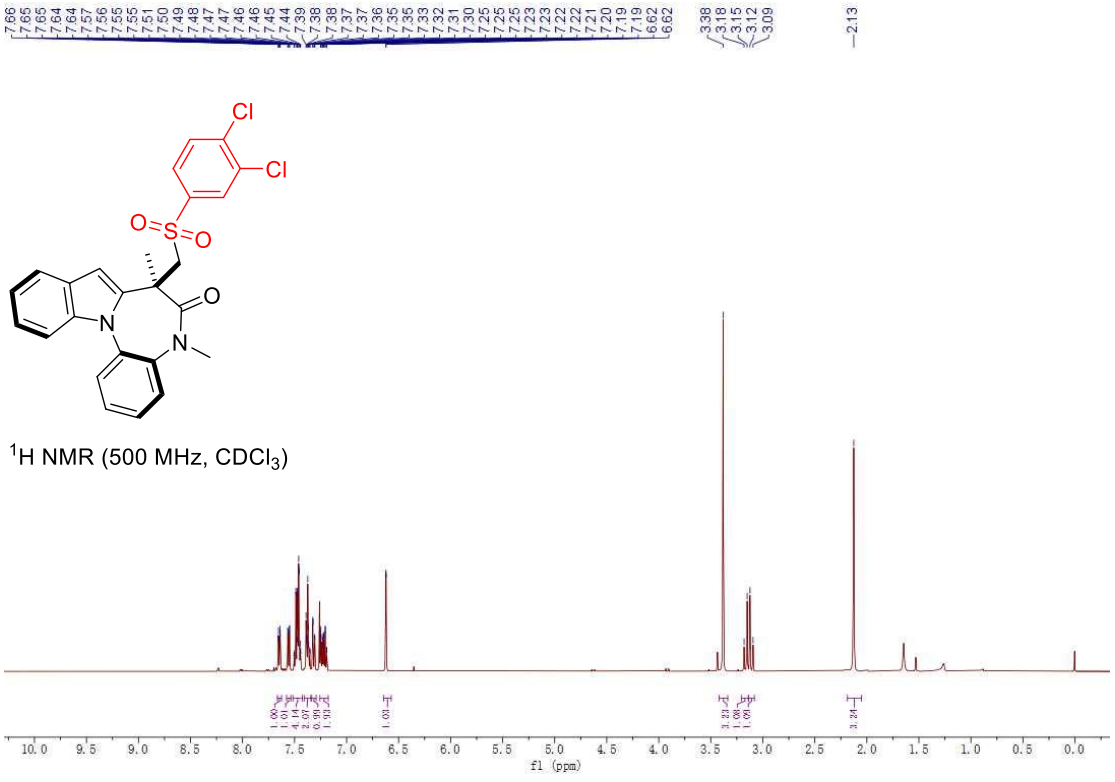
7-(((3,4-dimethylphenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5o)



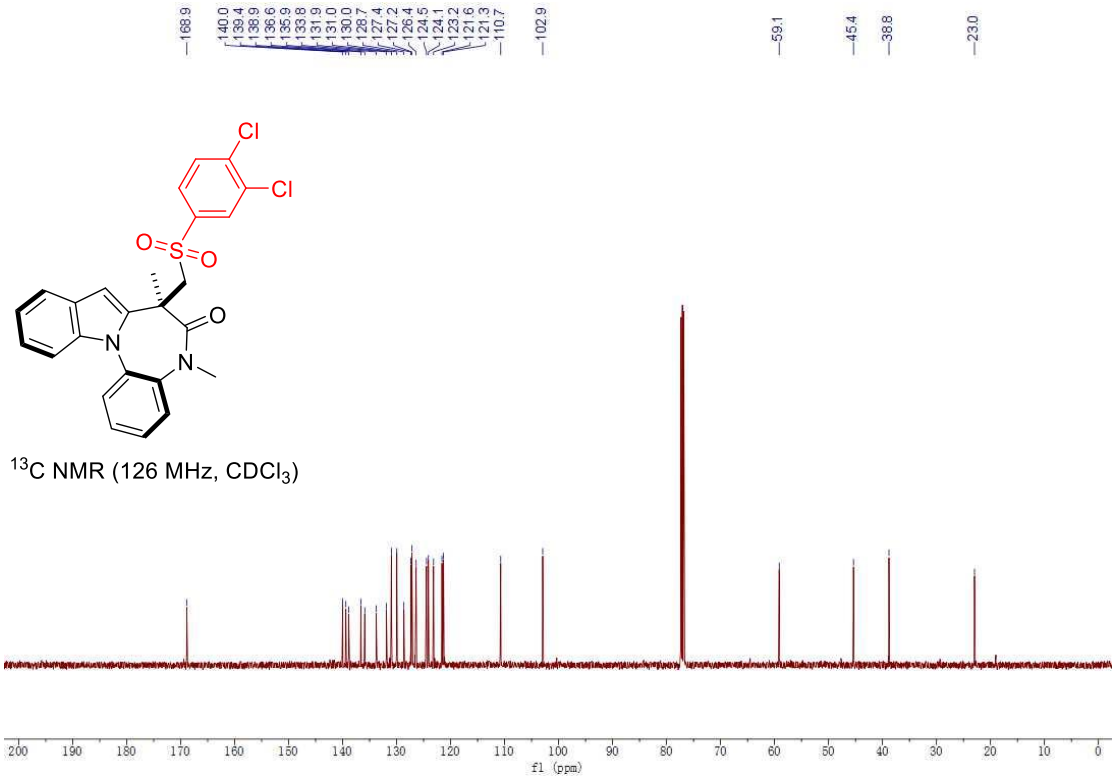
7-(((3,4-dimethylphenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5o)



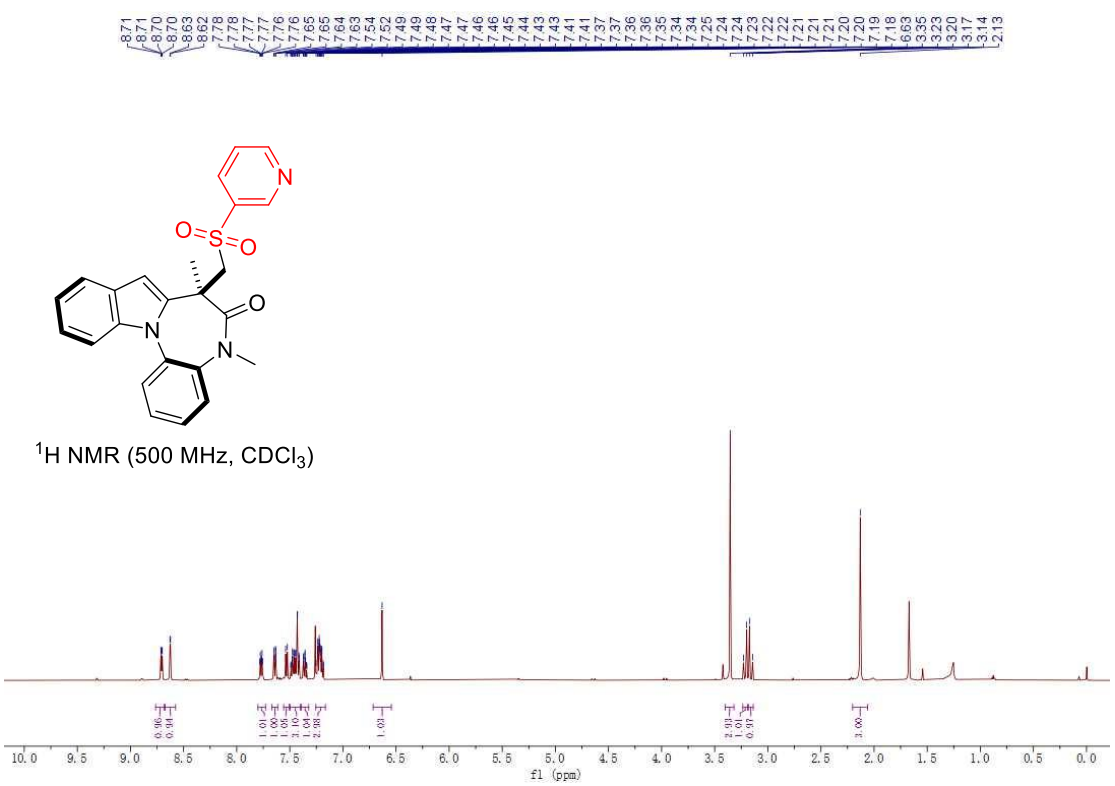
7-(((3,4-dichlorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5p)



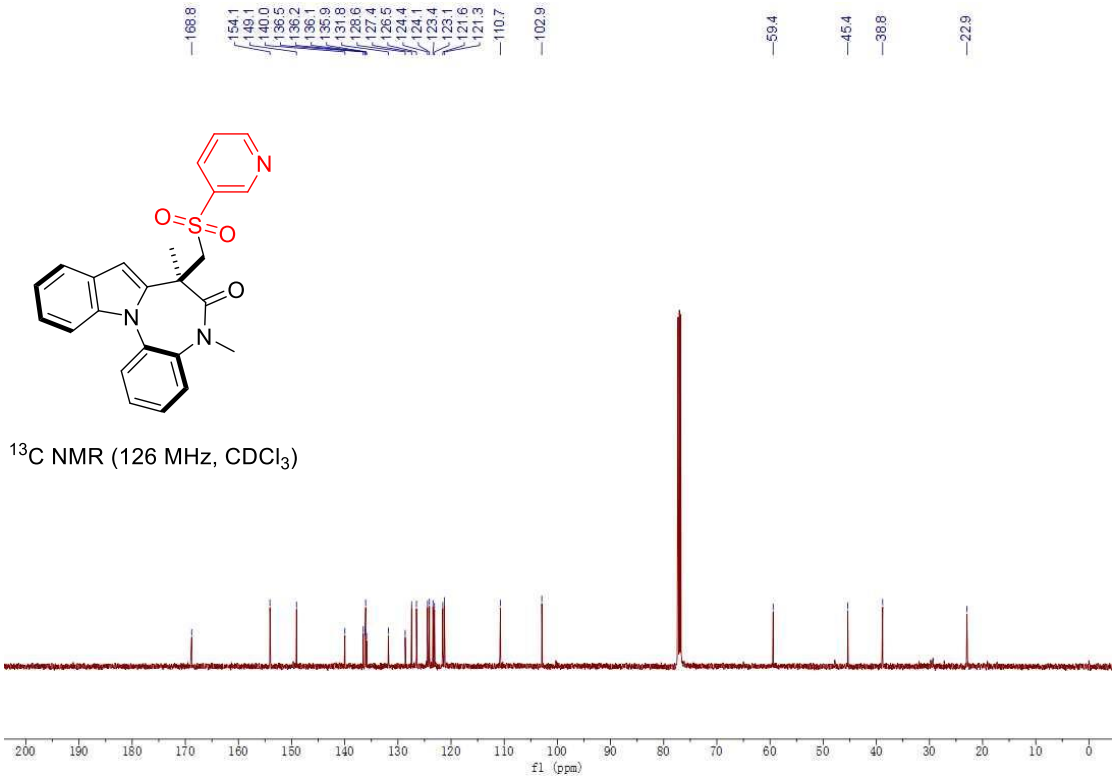
7-(((3,4-dichlorophenyl)sulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5p)



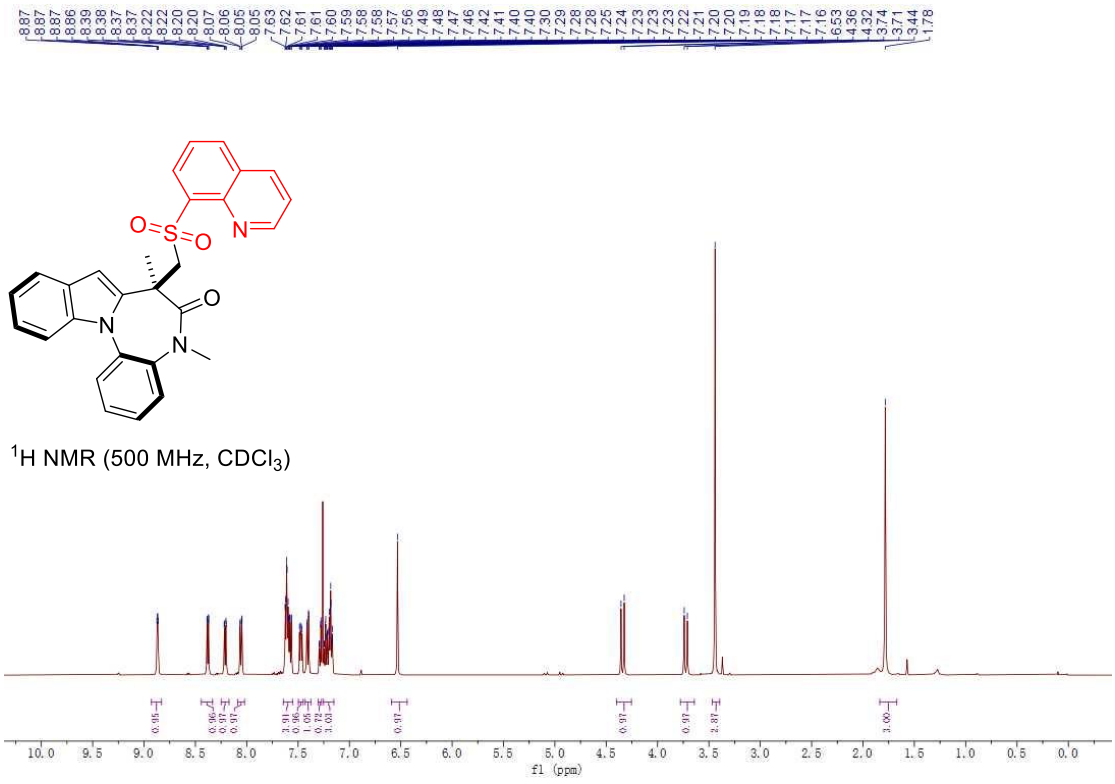
5,7-dimethyl-7-((pyridin-3-ylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5q)



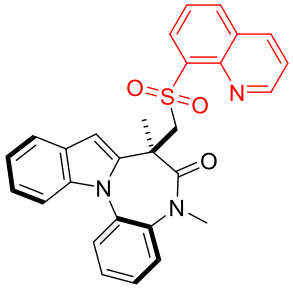
5,7-dimethyl-7-((pyridin-3-ylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5q)



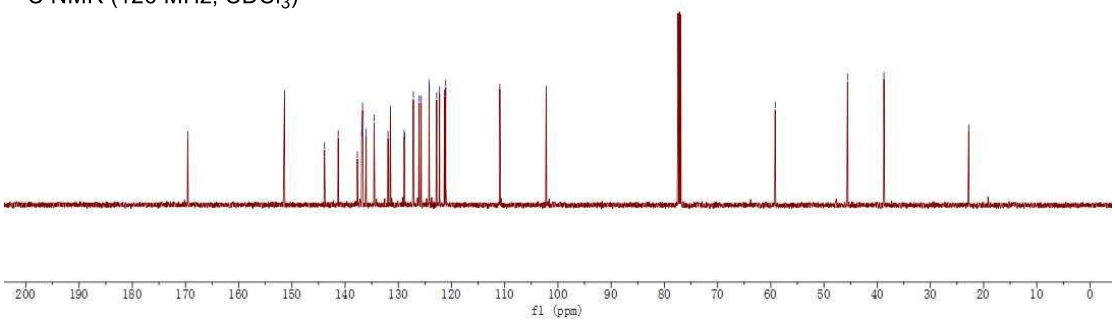
5,7-dimethyl-7-((quinolin-8-ylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5r)



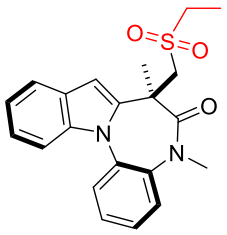
5,7-dimethyl-7-((quinolin-8-ylsulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5r)



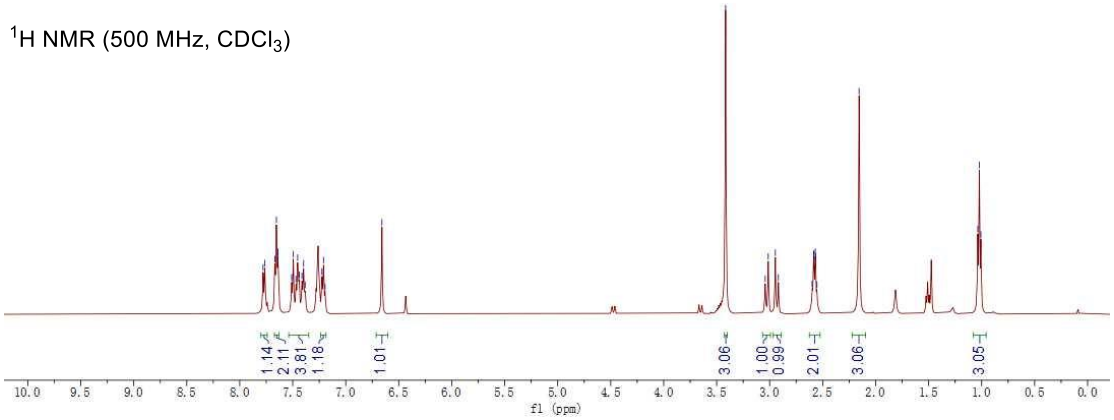
^{13}C NMR (126 MHz, $CDCl_3$)



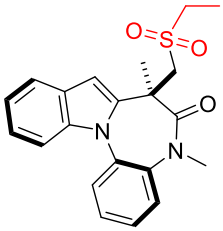
7-((ethylsulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5s)



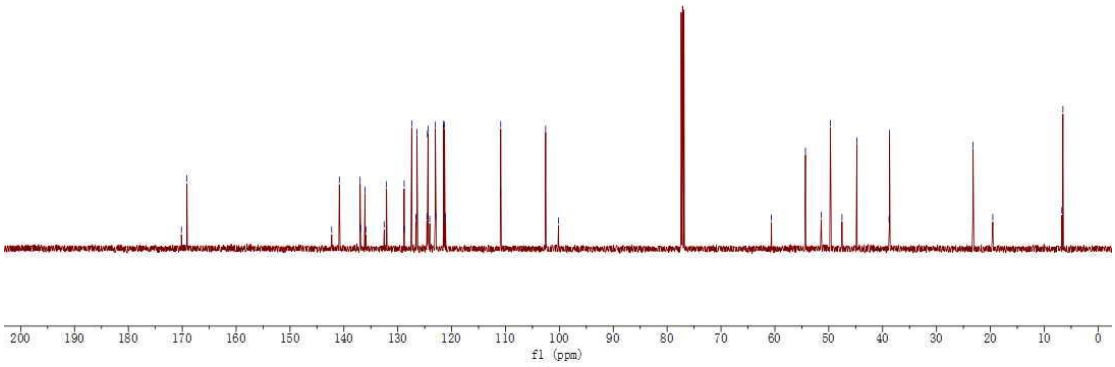
^{1}H NMR (500 MHz, $CDCl_3$)



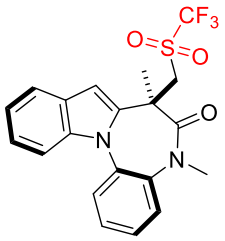
7-((ethylsulfonyl)methyl)-5,7-dimethyl-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5s)



^{13}C NMR (126 MHz, $CDCl_3$)

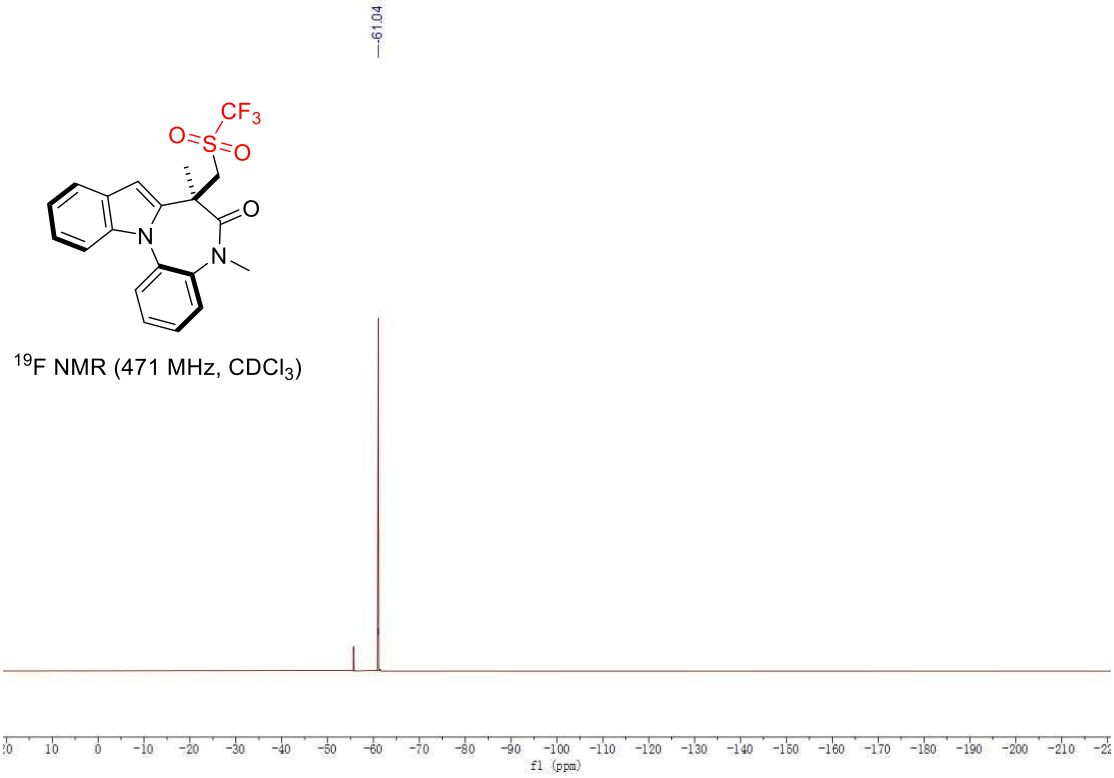


5,7-dimethyl-7-(((trifluoromethyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5t)



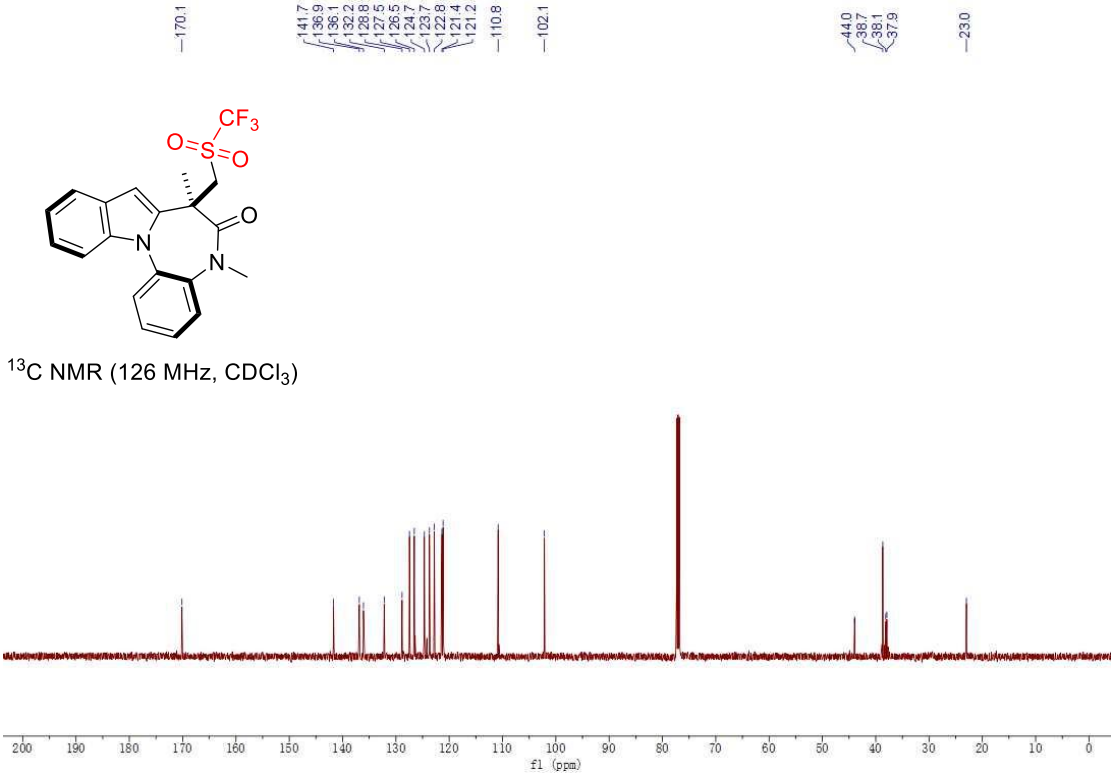
^{1}H NMR (500 MHz, $CDCl_3$)

5,7-dimethyl-7-(((trifluoromethyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5t)



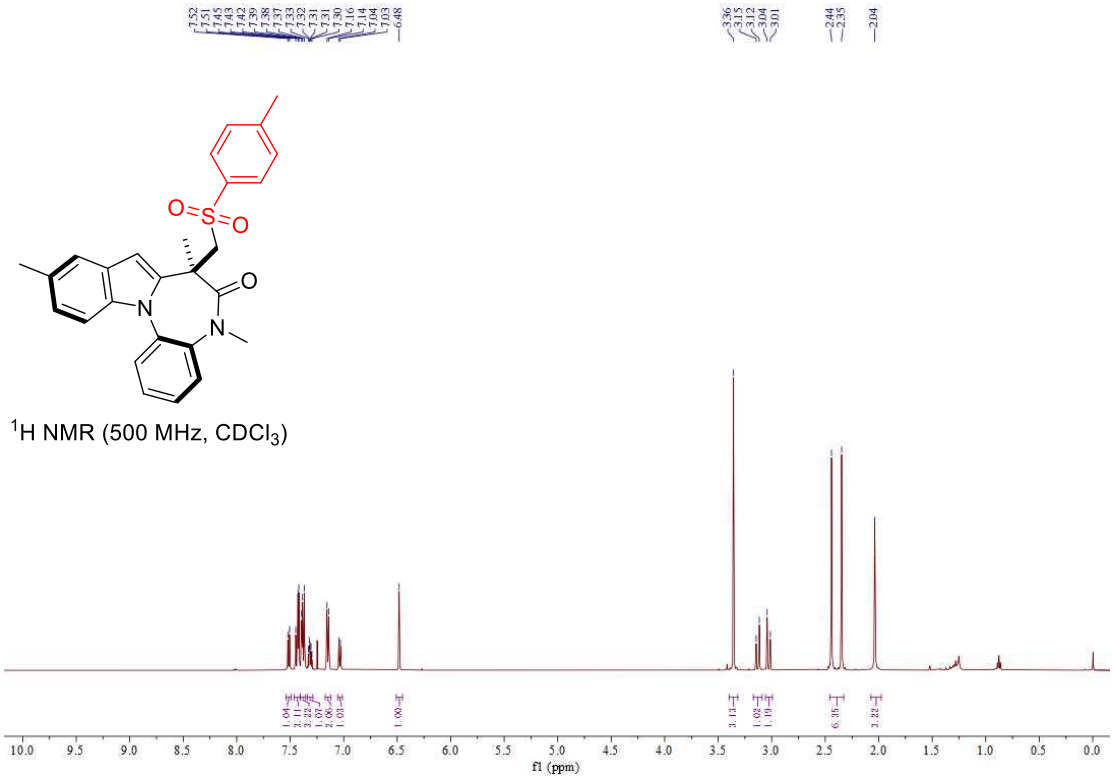
^{19}F NMR (471 MHz, $CDCl_3$)

5,7-dimethyl-7-(((trifluoromethyl)sulfonyl)methyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5t)

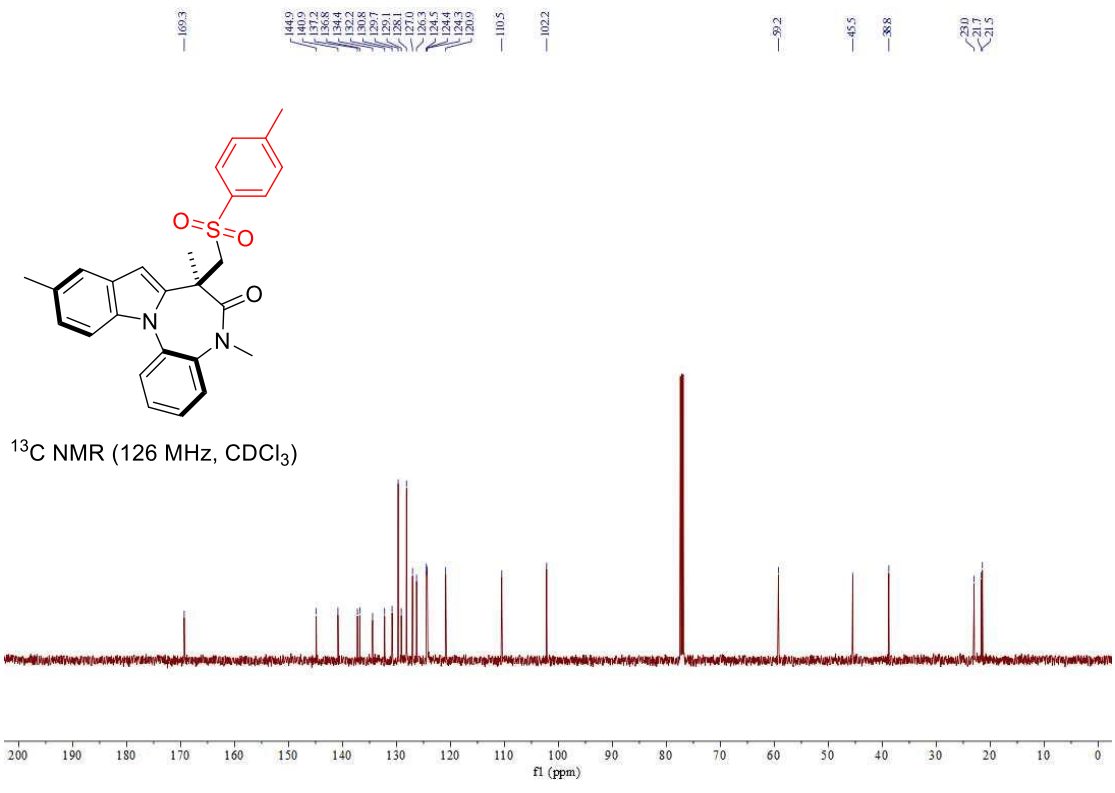


^{13}C NMR (126 MHz, $CDCl_3$)

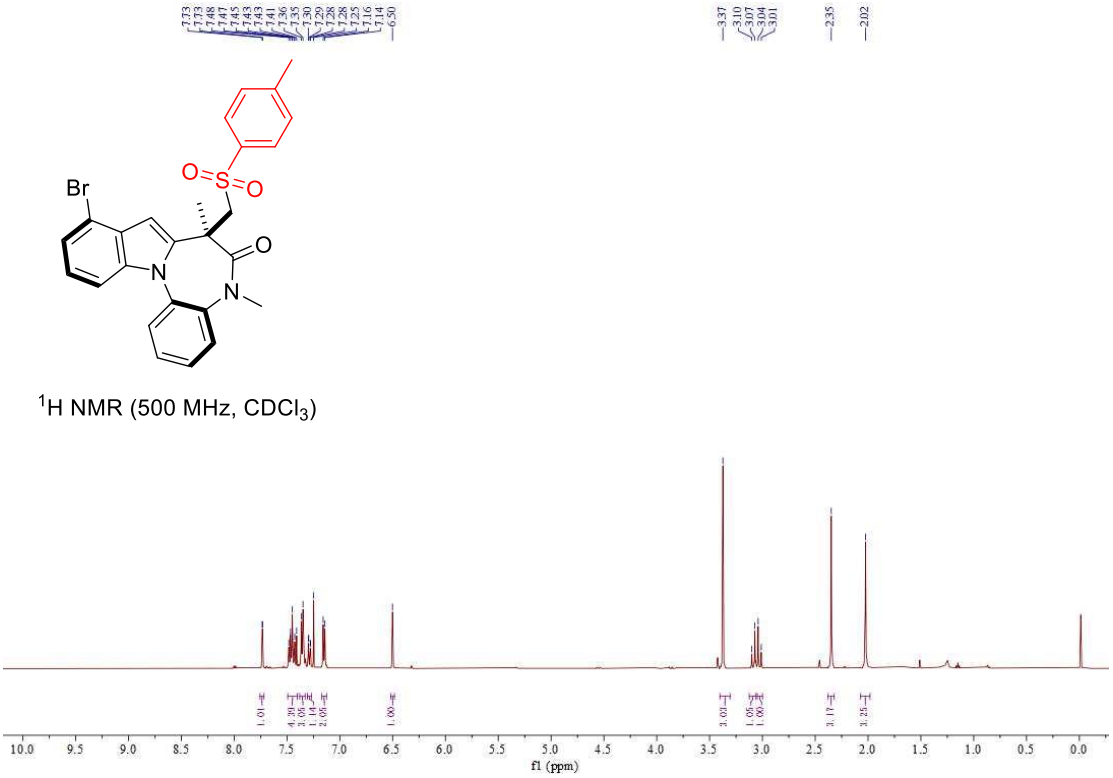
5,7,10-trimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5u)



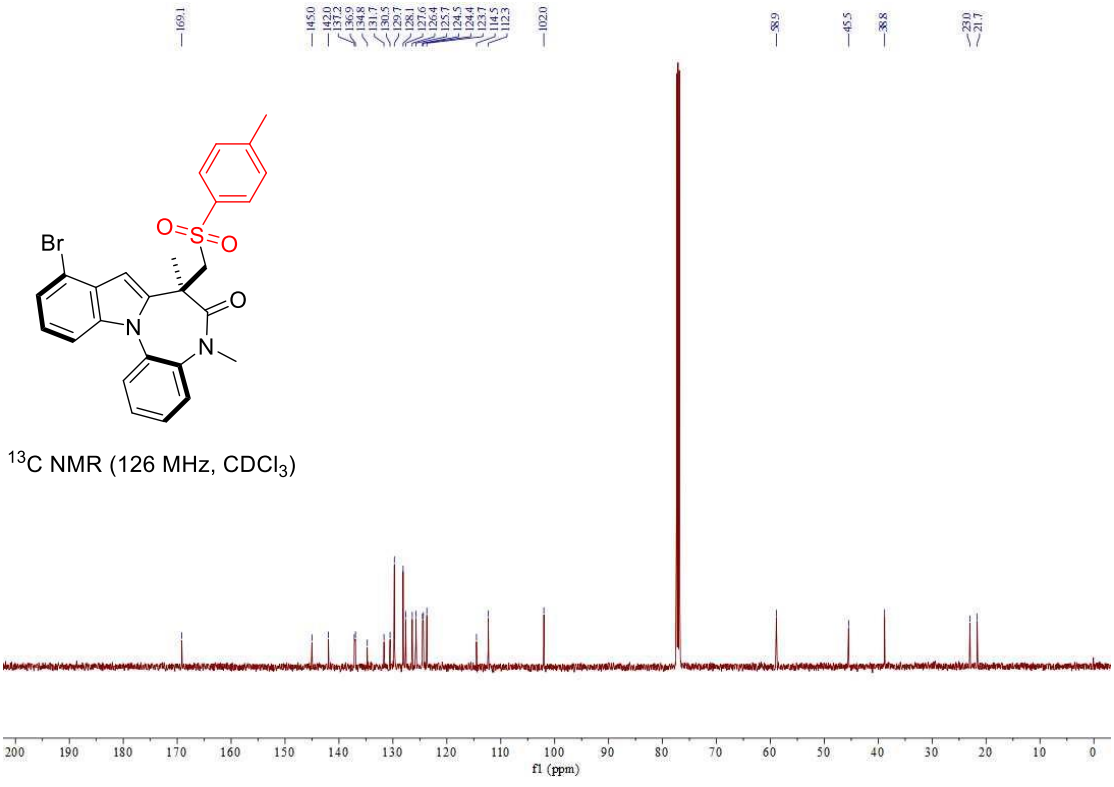
5,7,10-trimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5u)



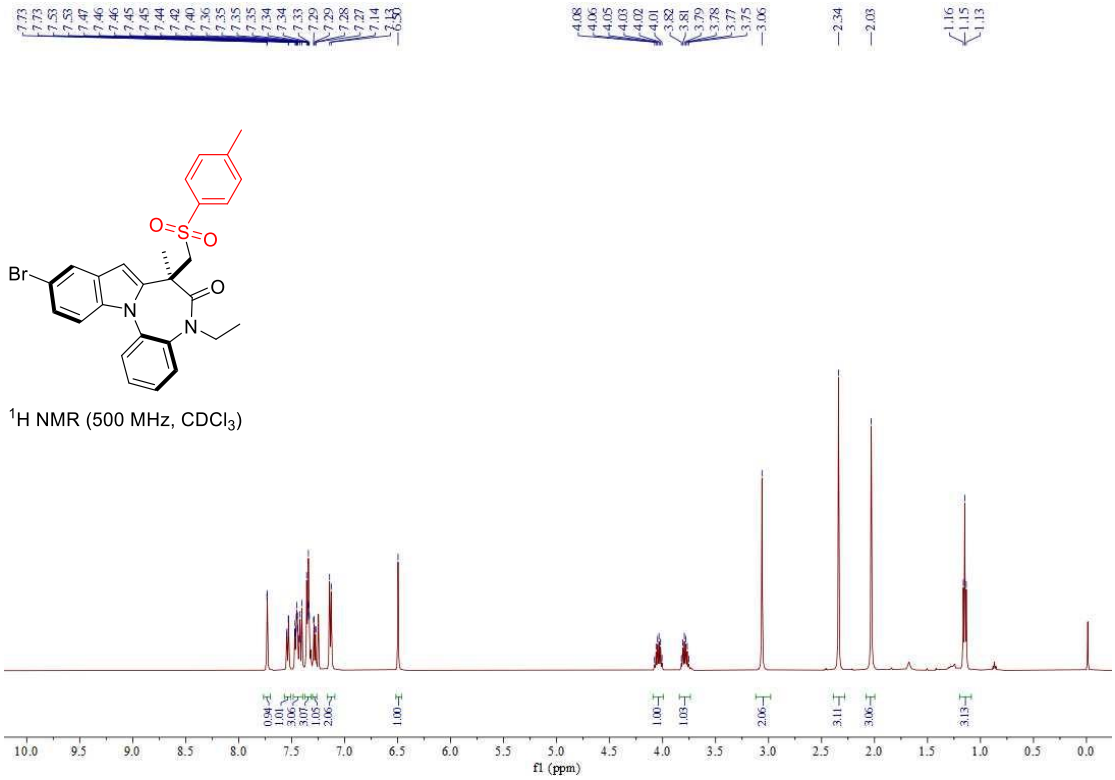
2-bromo-5,7-dimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5v)



2-bromo-5,7-dimethyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5v)



10-bromo-5-ethyl-7-methyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5w)



10-bromo-5-ethyl-7-methyl-7-(tosylmethyl)-5*H*-benzo[2,3][1,4]diazepino[1,7-*a*]indol-6(7*H*)-one (5w)