# Supporting Information

**Construction of pyrazolo[5,1-a]isoindol-8(3aH)-one derivatives via phosphine-catalyzed cyclization of electron-deficient alkynes and N-amino substituted phthalimide**

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## General information:

All reactions were performed in anhydrous solvents under an $N_2$ atmosphere. THF, $Et_2O$, and toluene were distilled from K and Na metal, respectively. DMF, $CH_2Cl_2$ and acetone were distilled from $CaH_2$. $CH_3CN$ was distilled from $P_2O_5$. PE refers to petroleum ether (boiling range 60–90 °C). Ethyl propiolate, methyl propiolate, dimethyl but-2-ynedioate and but-3-yn-2-one are commercially available without further purification. Other alkynoates[1] and alkyne ketones[2] were prepared following known procedures. N-(1,3-Dioxoisoindolin-2-yl)-sulfonamide(N-amino substituted phthalimide was prepared following known procedures.[3] Reaction progress was monitored using thin layer chromatography (TLC), which was visualized by ultraviolet light (254 nm). Flash chromatography was conducted with silica gel 200–300 mesh. Melting points were obtained on a Yanaco-241 apparatus and are uncorrected. $^1H$ and $^{13}C$ NMR spectra were recorded in DMSO-d6 using a Bruker Avance 300 spectrometer: chemical shifts (δ) are given in parts per million, coupling constants (*J*) in Hz. High-resolution mass spectra were recorded on a Waters/Micromass QTOF MS spectrometer.

## General procedure for reaction of electron-deficient alkynes with N-hydroxyphthalimide:

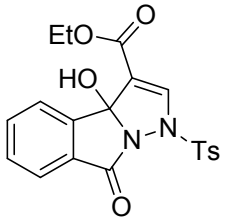
General experimental conditions: To the solution of electron-deficient alkyne (0.36 mmol) and N-(1,3-dioxoisoindolin-2-yl)-4-methylbenzenesulfonamide (94.8 mg, 0.3 mmol) (94.8 mg, 0.3 mmol) in dry DMF (1 mL) was added $Ph_3P$ (15.7 mg, 0.06 mmol). The resulting mixture was stirred at room temperature under nitrogen atmosphere for the required period of time. After completion of the reaction as monitored by TLC, the reaction mixture was quenched with $CH_2Cl_2$ (15 mL), which was washed with water and brine successively, dried over $MgSO_4$, filtered, and concentrated in vacuo. Purification by flash chromatography ($SiO_2$; ethylacetate/PE, 1:6~1:1) yielded the desired products.

[1] M. Newcomb, N. Miranda, X. Huang, D. Crich, *J. Am. Chem. Soc.* **2000**, 122, 6128.

[2] B.G. Van den Hoven, B. El Ali, H. Alper, *J. Org. Chem.* **2000**, *65*, 4131.

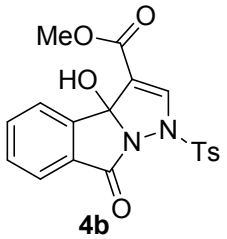
[3] O. M. A. Hafez, K. M. Amin, N. A. Abdel-Latif, T. K. Mohamed, E. Y. Ahmed, T. Maher *Eur. J. Med. Chem.* **2009**, *44*, 2957.

## Spectral data of the products:



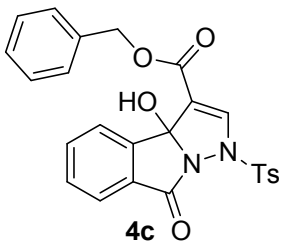
**4a**

White solid; m.p. 99-101 °C; $^1$H NMR (300 MHz, DMSO) δ 7.86-7.72 (m, 6H), 7.63-7.42 (m, 3H), 7.10 (s, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 2.41 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.50, 161.12, 145.97, 145.36, 142.31, 134.87, 131.05, 130.40, 129.71, 128.96, 127.96, 126.55, 123.86, 120.56, 97.28, 60.53, 21.19, 13.91; HRMS (ESI): calcd. for $C_{20}H_{18}N_2NaO_6S$ $[M+Na]^+$ 437.0778, found 437.0777.



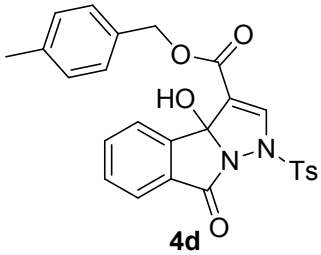
**4b**

White solid; m.p. 118-120 °C ; $^1$H NMR (300 MHz, DMSO) δ 7.86-7.74 (m, 6H), 7.63-7.42 (m, 3H), 7.09 (s, 1H), 3.66 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.51, 161.56, 145.98, 145.38, 142.39, 134.93, 131.00, 130.41, 129.72, 128.96, 127.95, 126.49, 123.88, 120.25, 97.27, 51.69, 21.19; HRMS (ESI): calcd. for $C_{19}H_{16}N_2NaO_6S$ $[M+Na]^+$ 423.0621, found 423.0623.



**4c**

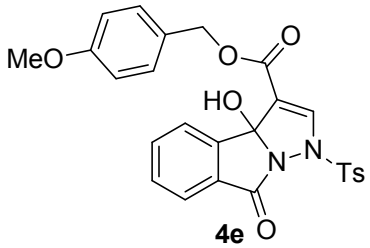
White solid; m.p. 97-99 °C ; $^1$H NMR (300 MHz, DMSO) δ 7.83-7.57 (m, 7H), 7.45-7.37 (m, 7H), 7.14 (s, 1H), 5.21-5.12 (m, 2H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.47, 160.95, 145.87, 145.39, 142.79, 135.62, 134.76, 131.03, 130.41, 129.70, 128.95, 128.39, 128.12, 128.06, 127.94, 126.55, 123.86, 120.22, 97.28, 65.91, 21.20; HRMS (ESI): calcd. for $C_{25}H_{20}N_2NaO_6S$ $[M+Na]^+$ 499.0934, found 499.0944.



**4d**

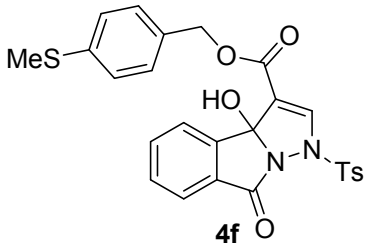
White solid; m.p. 97-99 °C ; $^1$H NMR (300 MHz, DMSO) δ 7.80-7.56 (m, 7H), 7.44-7.16 (m, 6H), 7.11 (s, 1H), 5.16-5.06 (m, 2H), 2.41 (s, 3H), 2.30 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.47, 160.96,

145.87, 145.38, 142.68, 137.50, 134.76, 132.56, 131.03, 130.40, 129.71, 128.94, 128.28, 127.93, 126.58, 123.85, 120.30, 97.27, 65.88, 21.19, 20.72; HRMS (ESI): calcd. for $C_{26}H_{22}N_2NaO_6S$ $[M+Na]^+$ 513.1091, found 513.1088.



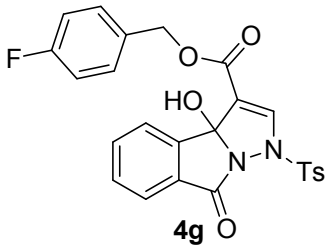

**4e**

White solid; m.p. 153-156 °C ; $^1$H NMR (300 MHz, DMSO) δ 7.79-7.57 (m, 7H), 7.44-7.31 (m, 4H), 7.10-6.92 (m, 3H), 5.11-5.05(m,2H), 3.75 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.45, 160.98, 159.25, 145.86, 145.36, 142.58, 134.72, 131.05, 130.38, 130.11, 129.69, 128.93, 127.93, 127.44, 126.59, 123.82, 120.37, 113.78, 97.26, 65.28, 55.08, 21.17; HRMS (ESI): calcd. for $C_{26}H_{22}N_2NaO_7S$ $[M+Na]^+$ 529.1040, found 529.1050.



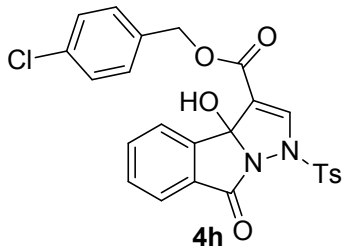

**4f**

White solid; m.p. 111-114 °C ; $^1$H NMR (300 MHz, DMSO) δ 7.79-7.58 (m, 7H), 7.44-7.25 (m, 6H), 7.11 (s, 1H), 5.14-5.08 (m, 2H), 2.47 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ172.45, 160.93, 145.86, 145.37, 142.73, 138.32, 134.76, 132.08, 131.03, 130.40, 129.69, 128.96, 128.93, 127.92, 136.54, 125.79, 123.84, 120.22, 97.25, 65.62, 21.18, 14.60; HRMS (ESI): calcd. for $C_{26}H_{22}N_2NaO_6S_2$[M+Na]$^+$ 545.0811, found 545.0817.



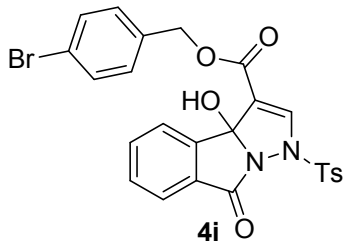

**4g**

White solid; m.p. 180-182 °C ; $^1$H NMR (300 MHz, DMSO) δ 7.82-7.57 (m, 7H), 7.47-7.17 (m, 6H), 7.12 (s, 1H), 5.19-5.10 (m, 2H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.47, 163.54 ($J_{CF}$ =195.75Hz), 160.30, 145.86, 145.40, 142.86, 134.77, 131.90($J_{CF}$ =2.25Hz), 131.04, 130.54, 130.43, 129.71, 128.95, 127.94, 126.54, 123.87, 120.15, 115.36($J_{CF}$ =21Hz), 97.27, 65.23, 21.19; HRMS (ESI): calcd. for $C_{25}H_{19}FN_2NaO_6S$ $[M+Na]^+$ 517.0840, found 517.0850.



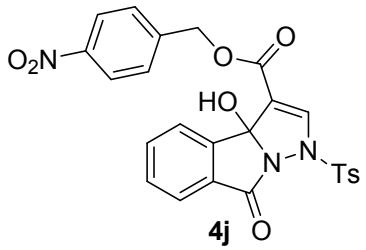

**4h**

White solid; m.p. 161-163 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.84-7.57 (m, 7H), 7.45-7.39 (m, 6H), 7.13 (s, 1H), 5.20-5.11 (m, 2H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.46, 160.89, 145.86, 145.39, 142.93, 134.79, 134.69, 132.77, 131.03, 130.43, 129.95, 129.71, 128.95, 128.38, 127.94, 126.50, 123.88, 120.05, 97.26, 65.08, 21.19; HRMS (ESI): calcd. for $C_{25}H_{19}ClN_2NaO_6S$ $[M+Na]^+$ 533.0545, found 533.0551.



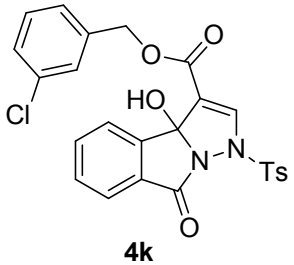

**4i**

White solid; m.p. 137-139 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.85-7.68 (m, 6H), 7.62-7.55 (m, 3H), 7.45-7.33 (m, 4H), 7.13 (s, 1H), 5.18-5.09 (m, 2H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.47, 160.89, 145.87, 145.40, 142.94, 135.11, 134.80, 131.31, 131.03, 130.43, 130.25, 129.71, 128.96, 127.94, 126.51, 123.89, 121.33, 120.05, 97.26, 65.12, 21.20; HRMS (ESI): calcd. for $C_{25}H_{19}BrN_2NaO_6S$ $[M+Na]^+$ 577.0039, found 577.0041.



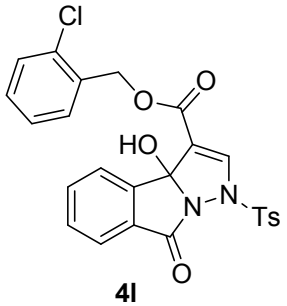

**4j**

Yellow solid; m.p. 149-151 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 8.26-7.75 (m, 8H), 7.70-7.46 (m, 5H), 7.18 (s, 1H), 5.34 (s, 2H), 2.44 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 172.48, 160.81, 147.14, 145.86, 145.43, 143.47, 143.22, 134.89, 131.04, 130.46, 129.73, 128.98, 128.62, 127.95, 126.47, 123.92, 123.47, 119.79, 97.28, 64.64, 21.19; HRMS (ESI): calcd. for $C_{25}H_{19}N_3NaO_8S$ $[M+Na]^+$ 544.0785, found 544.0785.



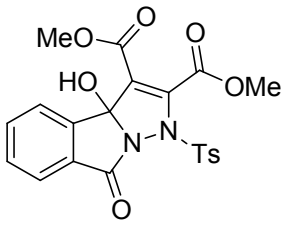

**4k**

White solid; m.p. 118-120 °C; $^1$H NMR (500 MHz, DMSO) δ 7.92 (s, 1H), 7.84 – 7.70 (m, 5H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.51 – 7.32 (m, 6H), 7.16 (s, 1H), 5.19 (q, *J* = 12.8 Hz, 2H), 2.43 (s, 3H); $^{13}$C NMR (125 MHz, DMSO) δ172.9, 161.4, 146.4 , 145.9 , 143.6 , 138.7 , 135.2 , 133.5 , 131.6 , 130.9 , 130.8, 130.2 , 129.4 , 128.5 , 128.2 , 127.0 , 124.4 , 120.5 , 97.8 , 65.5 , 21.7 ; HRMS (ESI): calcd. for $C_{25}H_{19}ClN_2NaO_6S$ $[M+Na]^+$ 533.0545, found 533.0546.



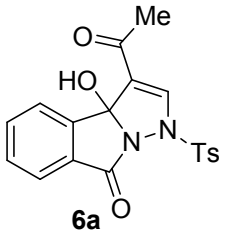

**4l**

White solid; m.p. 87-89 °C ; $^1$H NMR (500 MHz, DMSO) δ 7.87 (s, 1H), 7.82–7.80 (m, 3H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.68 (dd, *J* = 10.7, 4.2 Hz, 1H), 7.62–7.60 (m, 1H), 7.56–7.52 (m, 2H), 7.48–7.37 (m, 4H), 7.17 (s, 1H), 5.31 (d, *J* = 13.0 Hz, 1H), 5.23 (d, *J* = 13.0 Hz, 1H), 2.44 (s, 3H); $^{13}$C NMR (125 MHz, DMSO) δ172.9, 161.3, 146.3, 145.9, 143.5, 135.2, 133.5, 133.1, 131.5, 130.9, 130.8, 130.6, 130.2, 129.8, 129.4, 128.4, 127.8, 126.9, 124.4, 120.4, 97.8, 63.7, 21.7; HRMS (ESI): calcd. for $C_{25}H_{19}ClN_2NaO_6S$ $[M+Na]^+$ 533.0545, found 533.0557.



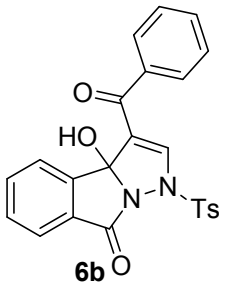

**4o**

White solid; m.p. 123-126 °C; $^1$H NMR (300 MHz, DMSO) δ 7.83-7.78 (m, 5H), 7.67-7.45 (m, 3H), 7.34 (s, 1H), 3.93 (s, 3H), 3.67 (s, 3H), 2.42 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 171.90, 160.56, 159.52, 145.93, 144.96, 144.35, 135.33, 130.83, 130.27, 129.79, 129.45, 127.96, 126.40, 124.13, 119.50, 97.25, 53.66, 52.33, 21.27; HRMS (ESI): calcd. for $C_{21}H_{22}N_3O_8S$ $[M+NH_4]^+$ 476.1122, found 476.1124.



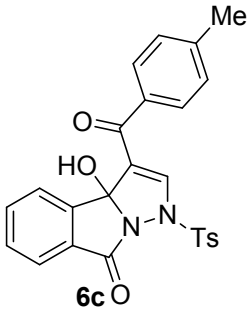

**6a**

White solid; m.p. 118-121 °C ; $^1$H NMR (300 MHz, DMSO) δ 8.16 (s, 1H), 7.92-7.72 (m, 5H), 7.60-7.41 (m, 3H), 6.85 (s, 1H), 2.40 (s, 3H), 2.26 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ191.89, 172.57, 146.31, 145.27, 144.09, 134.70, 131.08, 130.18, 129.68, 128.95, 128.03, 127.00, 123.60, 97.71, 27.48, 21.20; HRMS (ESI): calcd. for $C_{19}H_{16}N_2NaO_5S$ $[M+Na]^+$ 407.0672, found 407.0679.



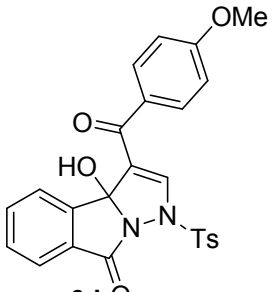

**6b**

White solid; m.p. 190-192 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.93-7.76 (m, 5H), 7.65-7.44 (m, 9H), 7.11 (s, 1H), 2.42 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 188.33, 172.42, 146.18, 145.48, 143.74, 138.14, 134.80, 132.56, 131.15, 130.34, 129.75, 129.05, 128.67, 128.44, 128.12, 126.77, 125.95, 123.79, 98.31, 21.21; HRMS (ESI): calcd. for $C_{24}H_{18}N_2NaO_5S$ $[M+Na]^+$ 469.0829, found 469.0827.



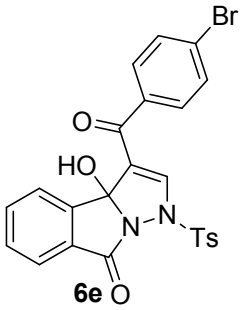

**6c**

White solid; m.p. 177-180 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.91-7.76 (m, 5H), 7.62-7.31 (m, 8H), 7.08 (s, 1H), 2.42 (s, 3H), 2.38 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 187.89, 172.42, 146.21, 145.44, 143.16, 142.94, 135.54, 134.75, 131.17, 130.30, 129.71, 129.18, 129.03, 128.59, 128.10, 126.73, 126.02, 123.76, 98.30, 21.19, 21.03; HRMS (ESI): calcd. for $C_{25}H_{20}N_2NaO_5S$ $[M+Na]^+$ 483.0985, found 483.0988.



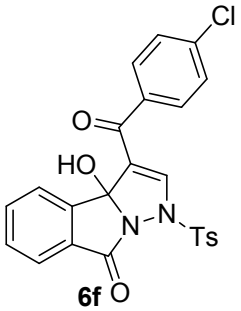

**6d**

White solid; m.p. 165-168 °C ;$^{1}$H NMR (300 MHz, DMSO) δ 7.90-7.75 (m, 5H), 7.61-7.46 (m, 6H), 7.04 (s, 2H), 7.02 (s, 1H), 3.84 (s, 3H), 2.42 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 186.71, 172.44, 162.89, 146.27, 145.38, 142.18, 135.26, 134.71, 130.85, 130.26, 129.69, 129.05, 128.08, 127.37, 126.67, 126.05, 123.73, 113.91, 98.32, 55.49, 21.18. HRMS (ESI): calcd. for $C_{25}H_{20}N_2NaO_6S$ $[M+Na]^+$ 499.0934, found 499.0939.



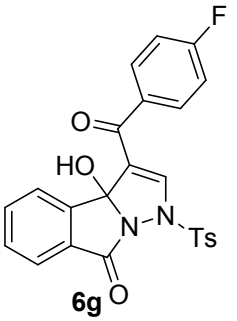

**6e**

White solid; m.p. 168-170 $^{o}$C ;$^{1}$H NMR (300 MHz, DMSO) δ 7.92-7.70(m, 8H), 7.63-7.44 (m, 5H), 7.10 (s, 1H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 187.43, 172.36, 146.09, 145.49, 144.44, 137.17, 134.81, 131.69, 131.17, 130.47, 130.35, 129.76, 129.02, 128.14, 126.71, 126.43, 125.69, 123.80, 98.23, 21.22; HRMS (ESI): calcd. for $C_{24}H_{17}BrN_2NaO_5S$ [M+Na]$^{+}$ 546.9934, found 546.9941.



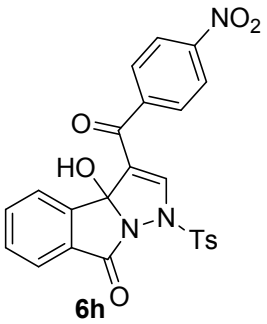

**6f**

White solid; m.p. 232-235 $^{o}$C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.92-7.69 (m , 6H), 7.63-7.44 (m, 7H), 7.10 (s, 1H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 187.25, 172.36, 146.09, 145.49, 144.36, 137.37, 136.83, 134.80, 131.17, 130.35, 129.75, 129.02, 128.74, 128.14, 126.70, 125.71, 123.80, 114.10, 98.24, 21.21; HRMS (ESI): calcd. for $C_{24}H_{17}ClN_2NaO_5S$ [M+Na]$^{+}$ 503.0439, found 503.0449.



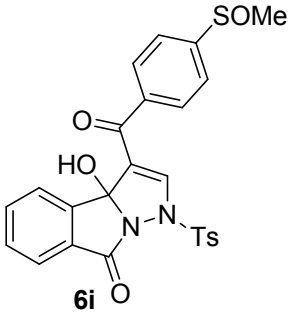

**6g**

White solid; m.p. 207-210 $^{o}$C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.90-7.75 (m, 5H), 7.71-7.58 (m, 4H), 7.47-7.30 (m, 4H), 7.09 (s, 1H), 2.42 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 186.95, 172.37, 166.26 ($J_{CF}$ = 249Hz), 146.13, 145.48, 143.87, 134.78, 134.73, 131.44 ($J_{CF}$ =9.75Hz), 131.17, 130.33, 129.74, 129.03, 128.13, 126.68, 125.81, 123.79, 115.82($J_{CF}$=22.5Hz), 98.26, 21.21; HRMS (ESI): calcd. for $C_{24}H_{17}FN_2NaO_5S$ [M+Na]$^{+}$ 487.0734, found 487.0750.



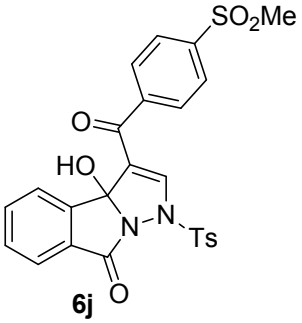

**6h**

Yellow solid; m.p. 167-171 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.92-7.69 (m, 8H), 7.63-7.44 (m, 5H), 7.09 (s, 1H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 187.39, 172.31, 146.06, 145.45, 144.34, 137.15, 134.75, 131.64, 131.18, 130.41, 130.30, 129.71, 128.98, 128.10, 126.67, 126.37, 125.66, 123.75, 98.19, 21.17; HRMS (ESI): calcd. for $C_{24}H_{17}N_3NaO_7S$ $[M+Na]^+$ 514.0679, found 514.0687.



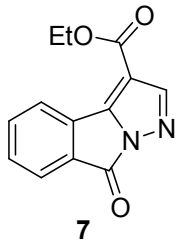

**6i**

White solid; m.p. 97-101 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 7.96-7.76 (m, 9H), 7.72-7.44 (m, 4H), 7.13 (s, 1H), 2.81 (s, 3H), 2.41 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 187.73, 172.39, 150.63, 146.10, 145.53, 144.74, 139.88, 134.84, 131.16, 130.38, 129.79, 129.18, 129.05, 128.17, 126.78, 125.82, 123.95, 123.84, 98.29, 42.96, 21.24; HRMS (ESI): calcd. for $C_{25}H_{21}N_2O_6S_2$ $[M+H]^+$ 509.0836, found 509.0840.




**6j**

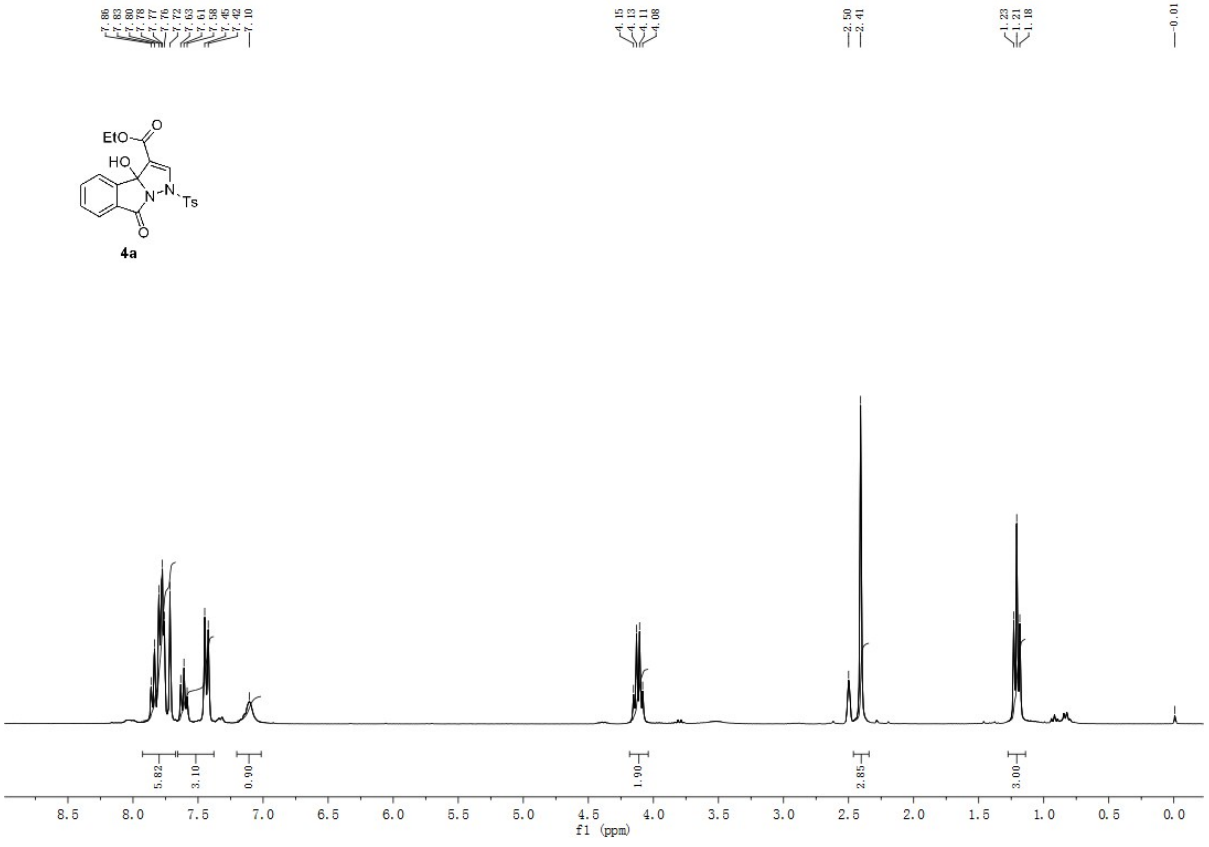
Yellow solid; m.p. 121-123 °C ; $^{1}$H NMR (300 MHz, DMSO) δ 8.06-7.79 (m, 9H), 7.74-7.46 (m, 5H), 7.14 (s, 1H), 3.28 (s, 3H), 2.42 (s, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 188.10, 172.83, 146.52, 146.05, 144.04, 142.71, 135.35, 131.66, 130.89, 130.30, 129.70, 129.51, 128.66, 127.83, 127.28, 126.21, 124.32, 98.70, 43.75, 21.72; HRMS (ESI): calcd. for $C_{25}H_{20}N_2NaO_7S_2$ $[M+Na]^+$ 547.0604, found 547.0610.

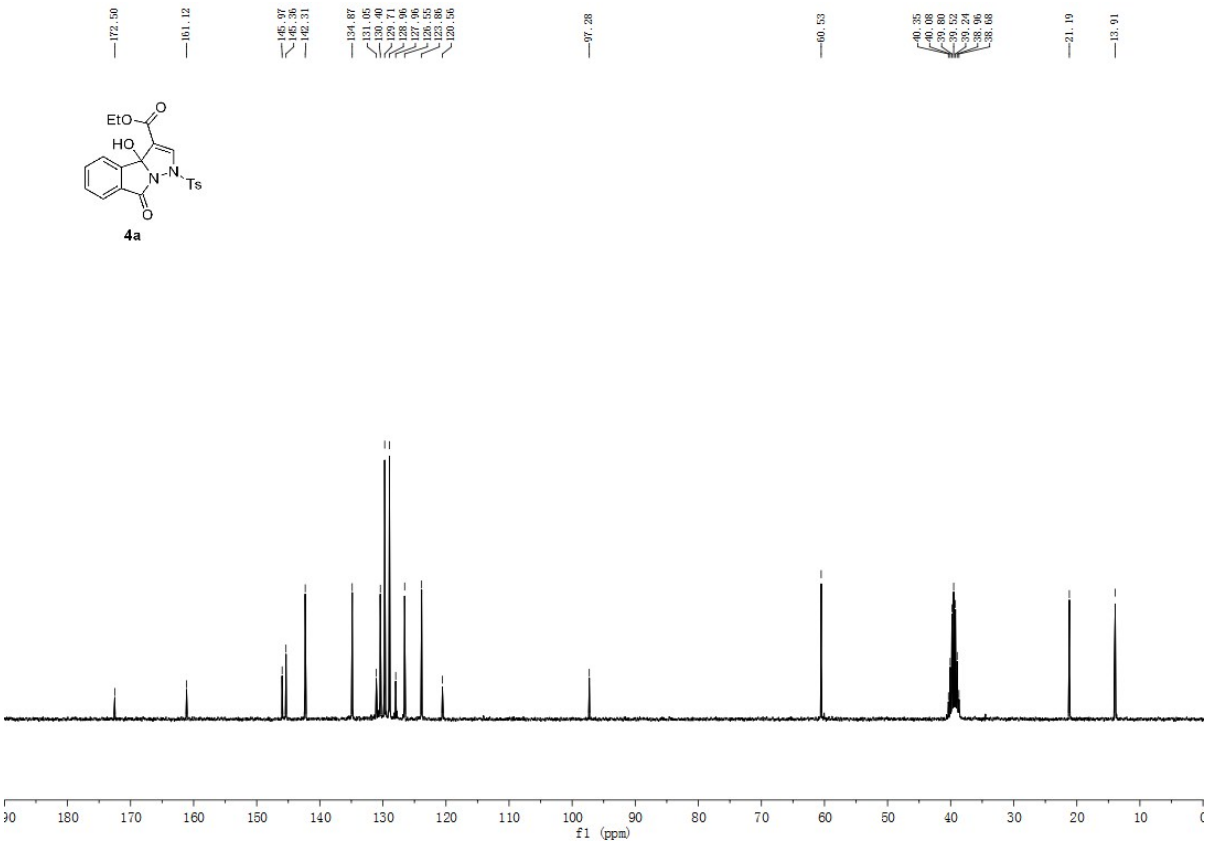



**7**

Yellow solid; m.p. 129-131 $^{o}$C; $^{1}$H NMR (300 MHz, DMSO) δ 8.12 (s, 1H), 7.93-7.81 (m, 2H), 7.78-7.54 (m, 2H), 4.39 (q, $J$ = 7.1 Hz, 2H), 1.39 (t, $J$ = 7.1 Hz, 3H); $^{13}$C NMR (75 MHz, DMSO) δ 161.21, 159.53, 148.76, 148.02, 135.77, 131.36, 130.59, 130.06, 126.54, 124.13, 111.05, 60.97, 14.17; HRMS (ESI): calcd. for $C_{13}H_{11}N_2O_3$ $[M+H]^+$ 243.0764, found 243.0769.

## Copies of $^{1}$HNMR and $^{13}$CNMR spectra:

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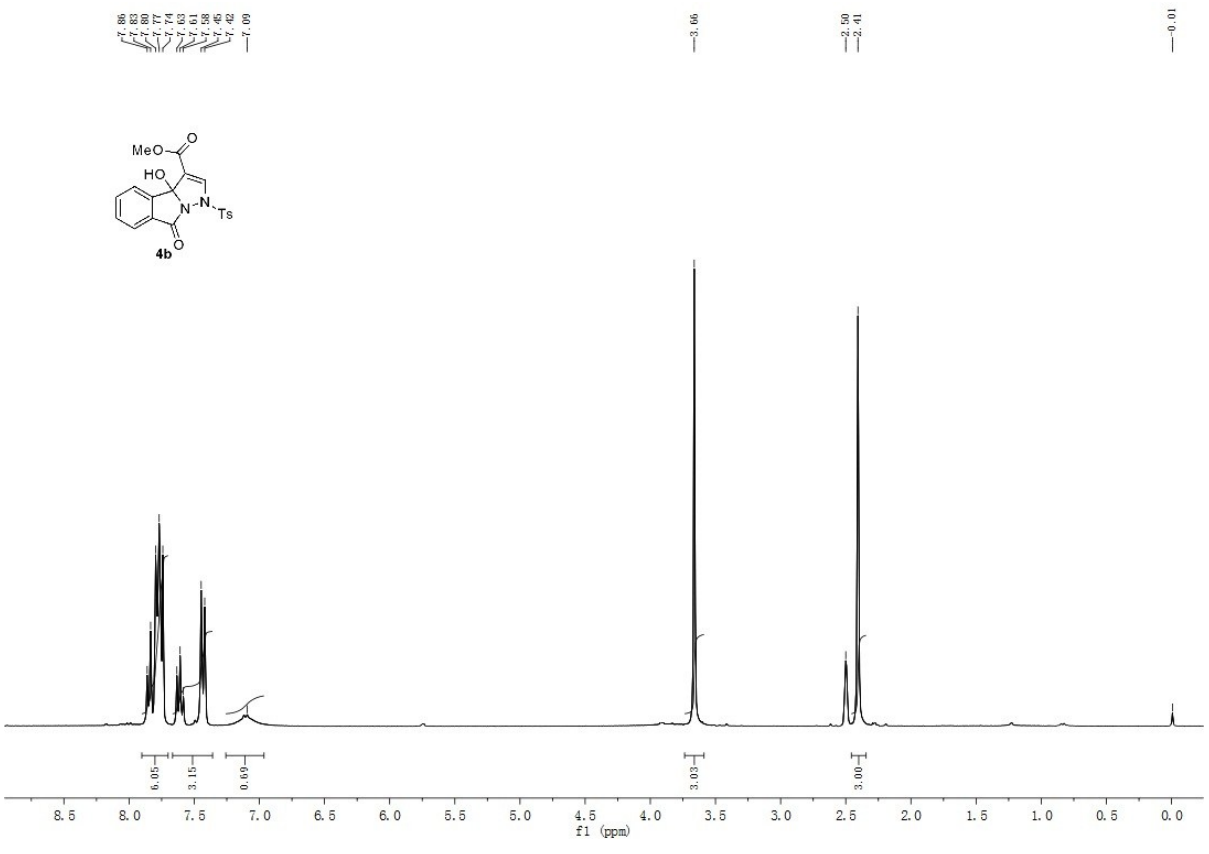
N
Ts
O
O
4a
f1 (ppm)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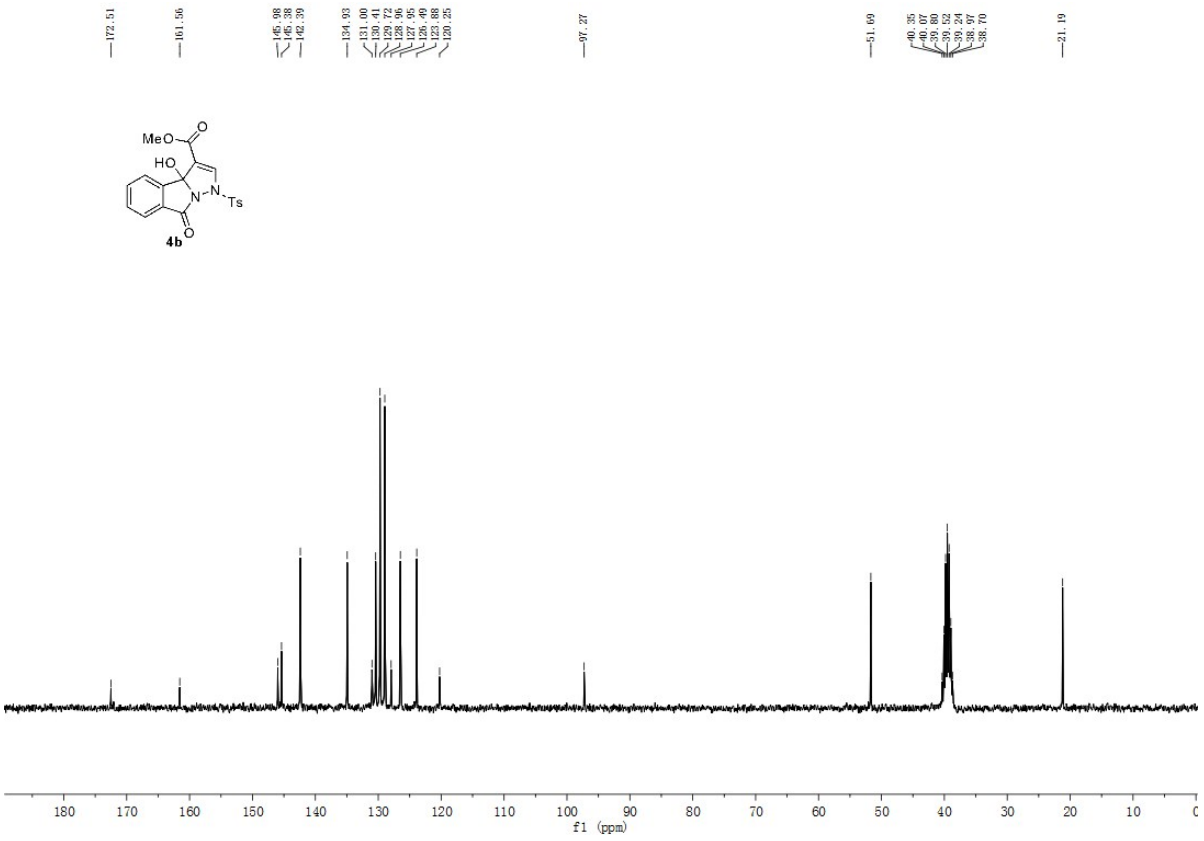
f1 (ppm)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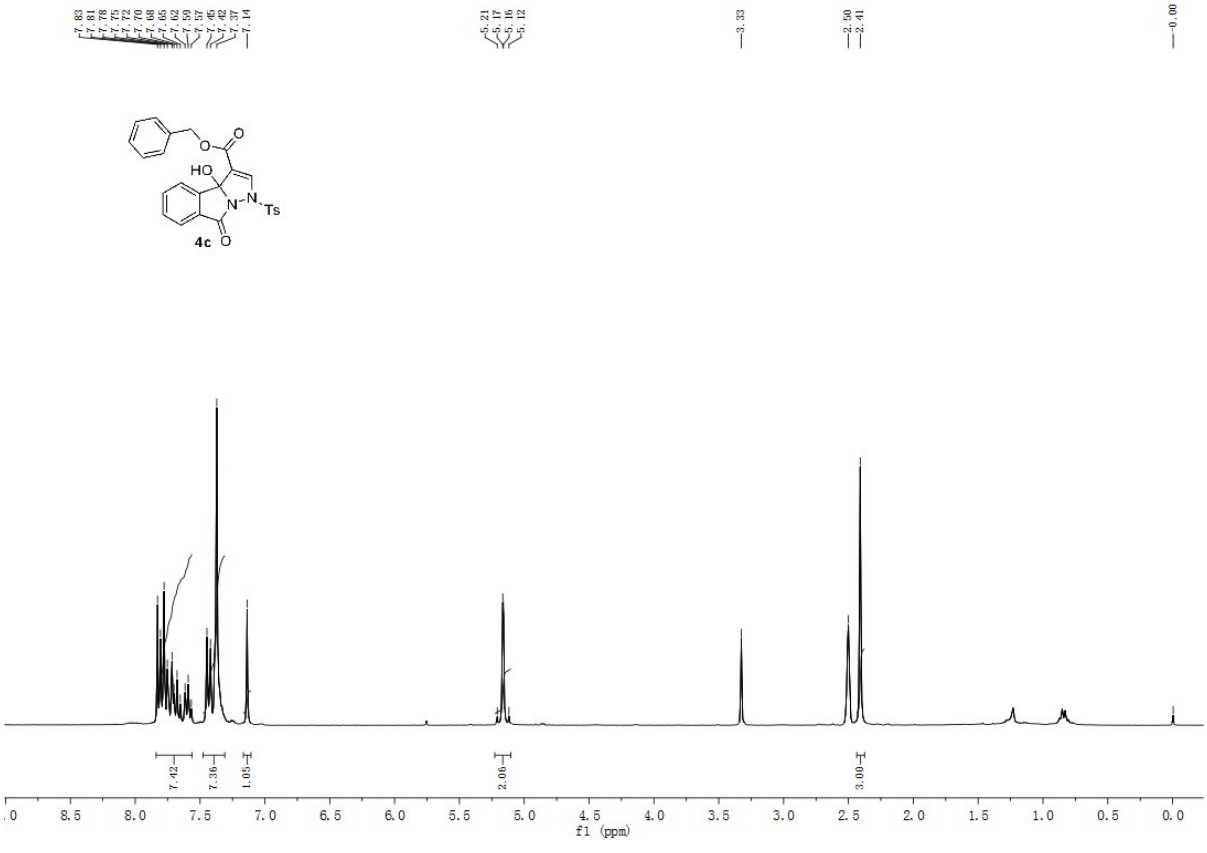
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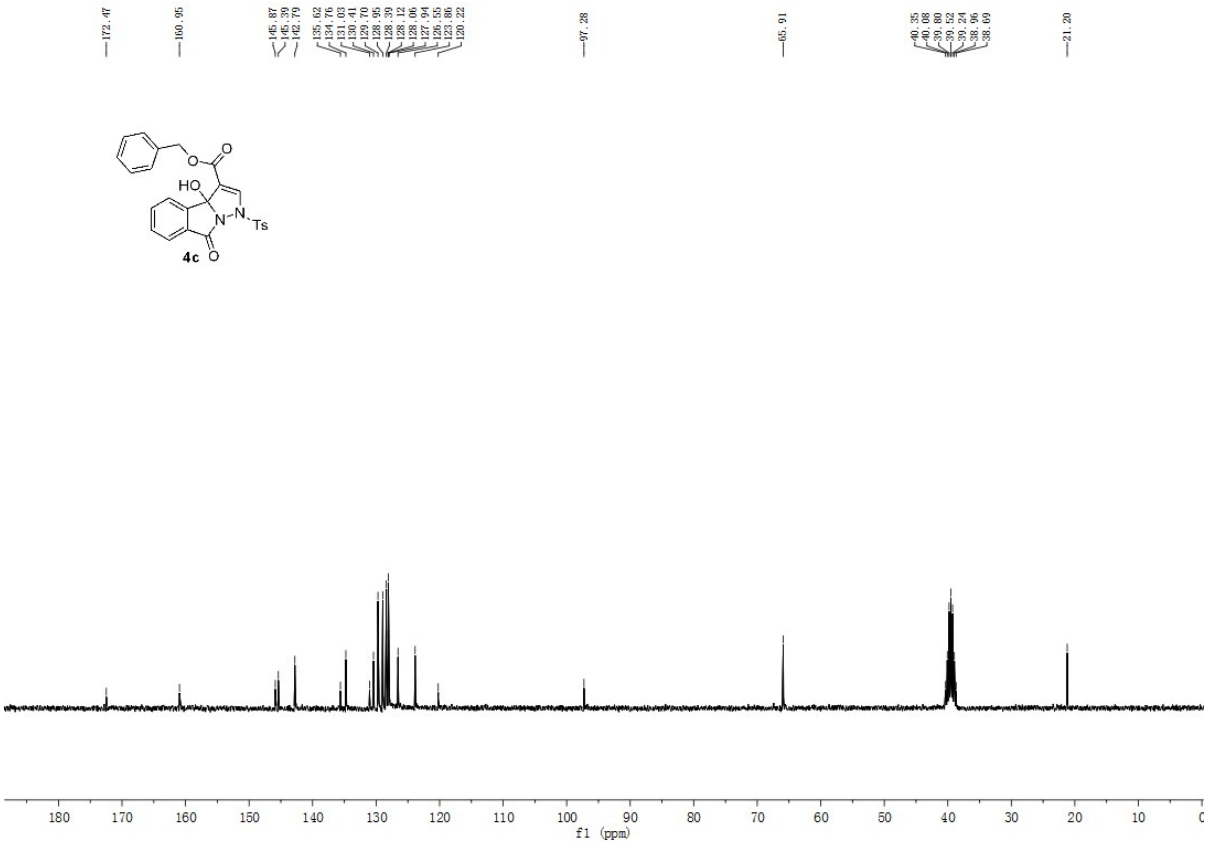
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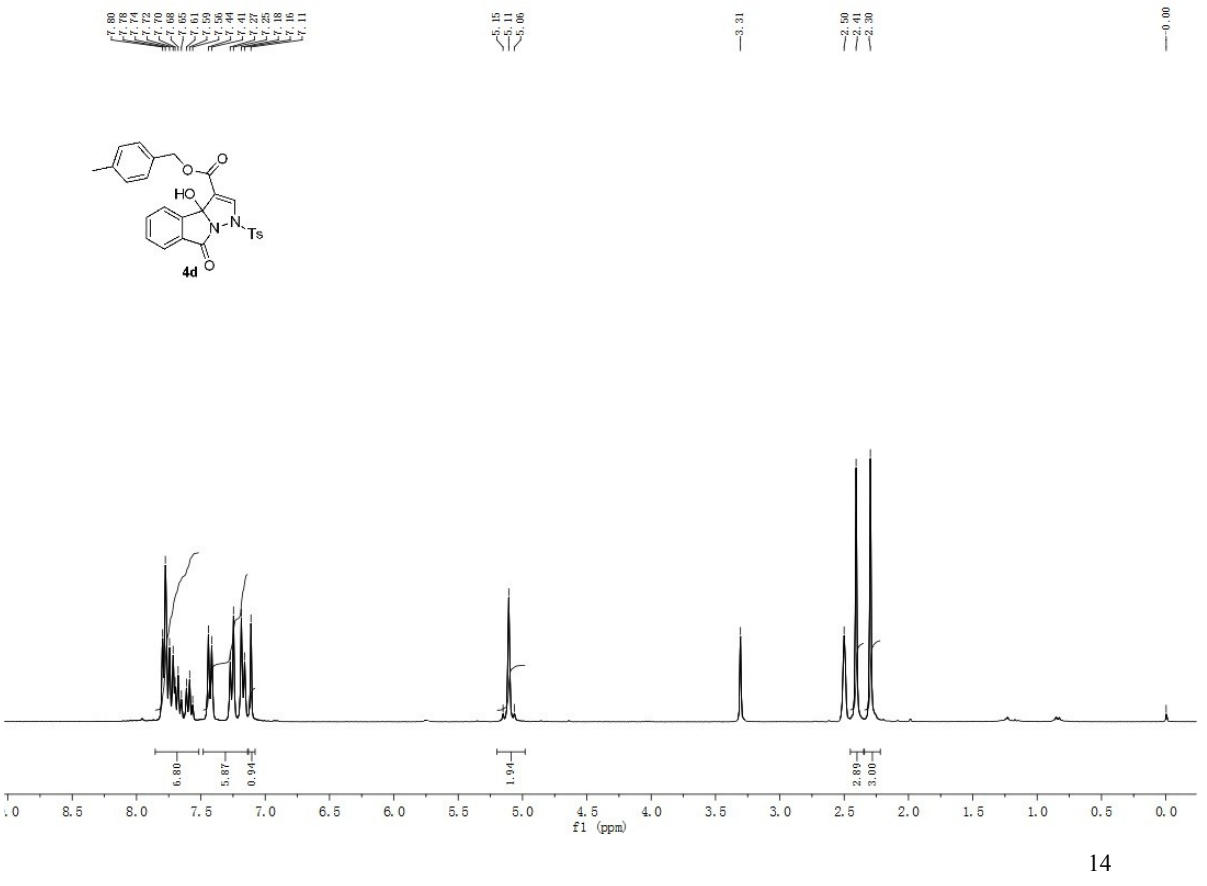
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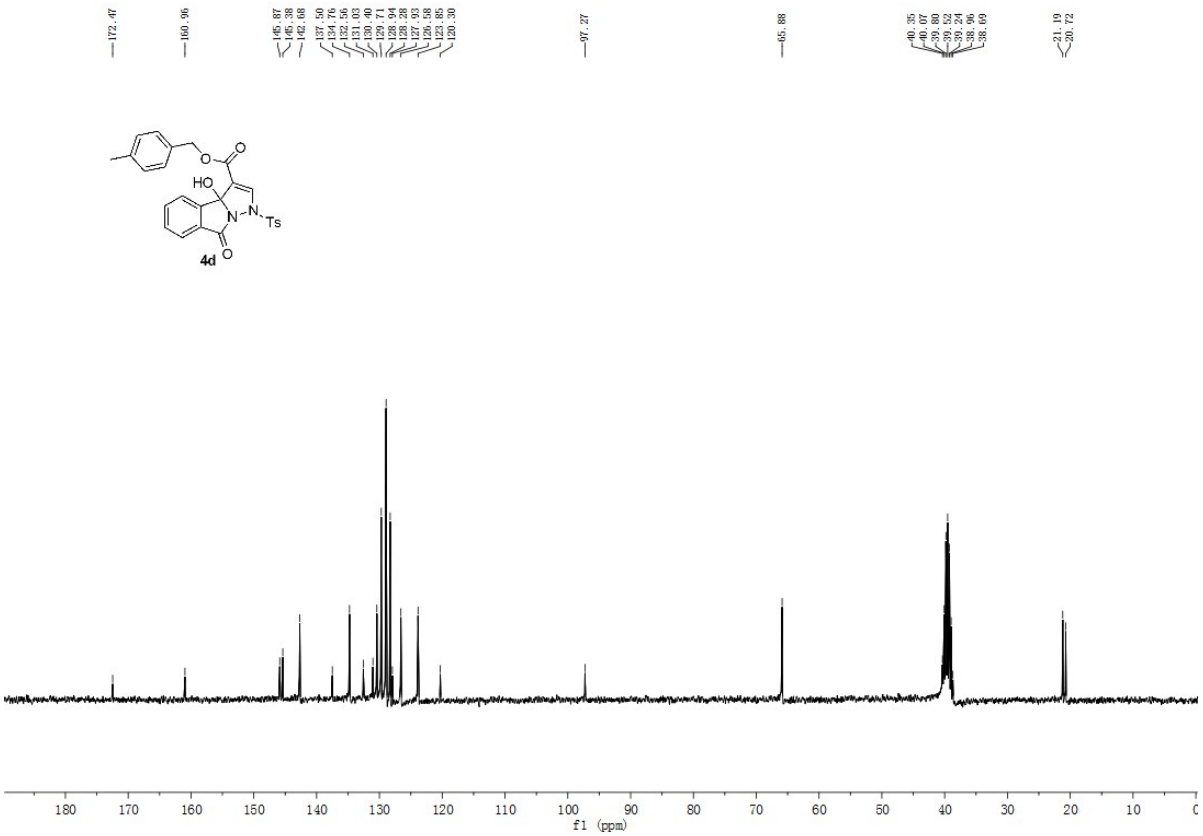
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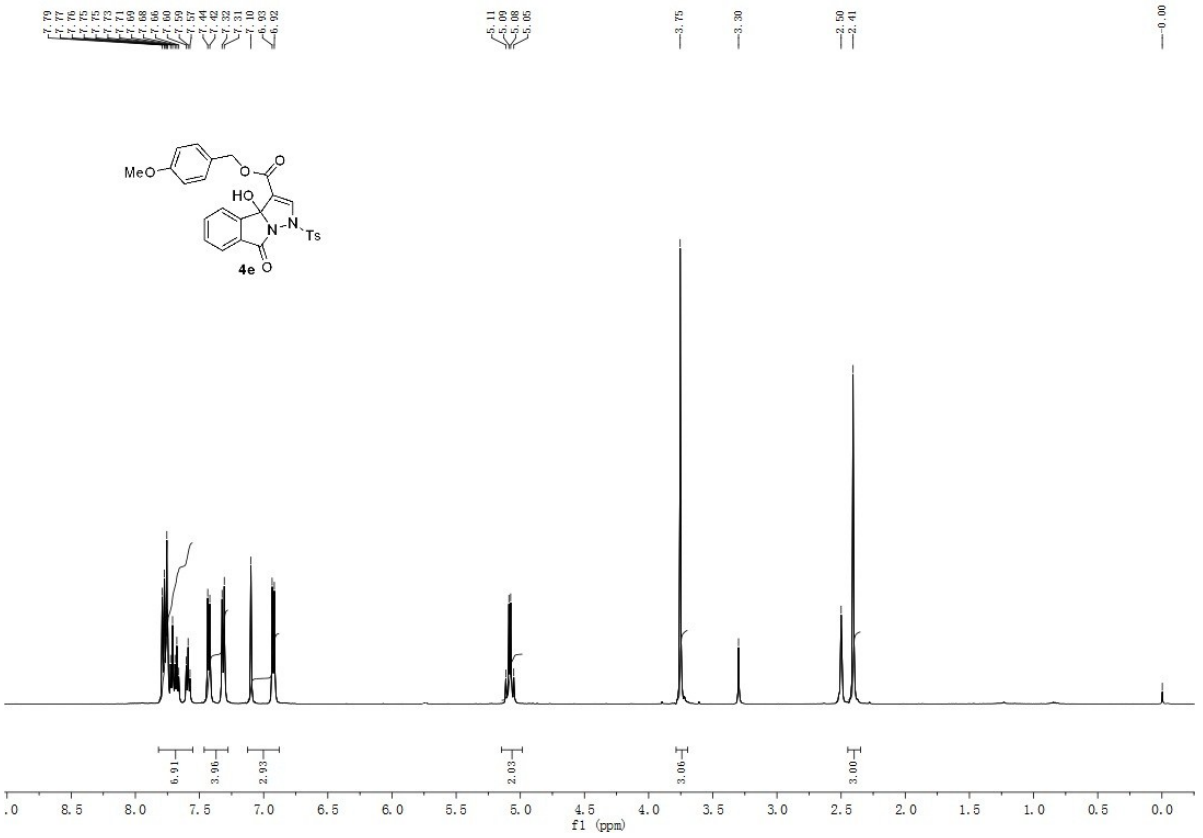
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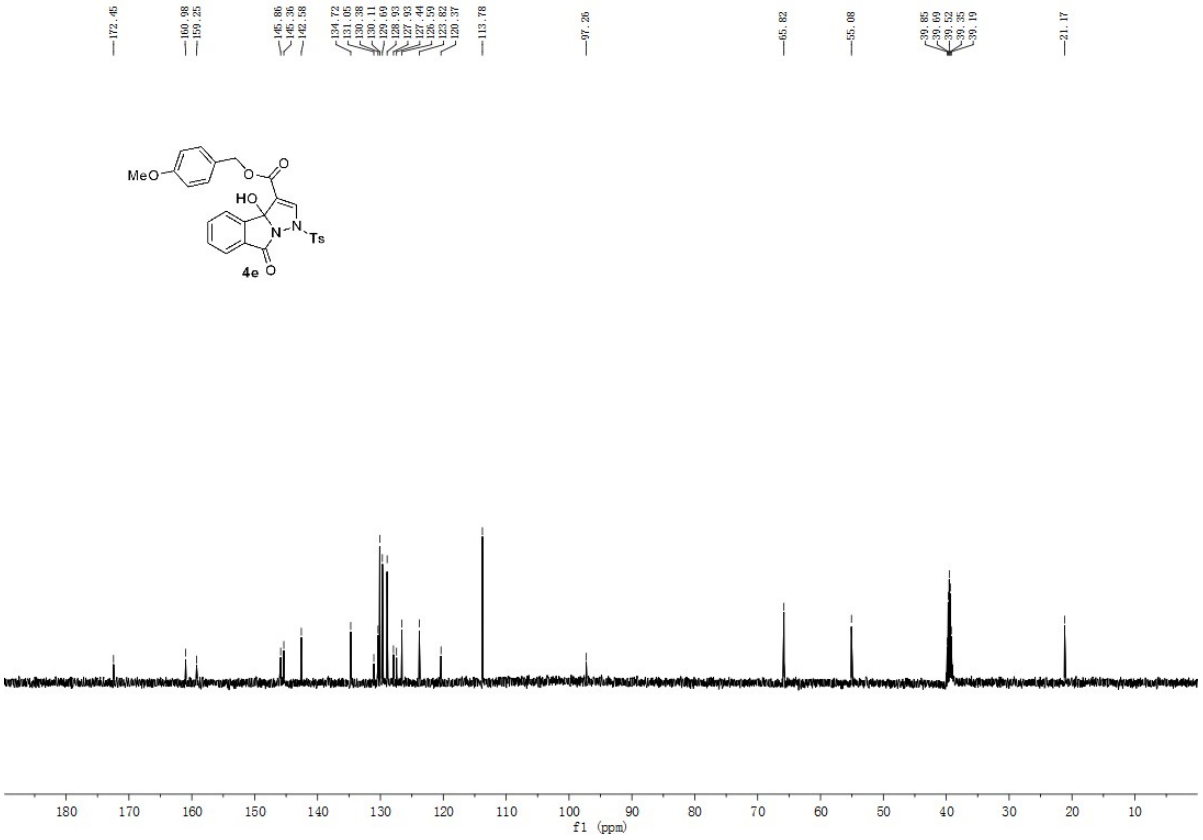
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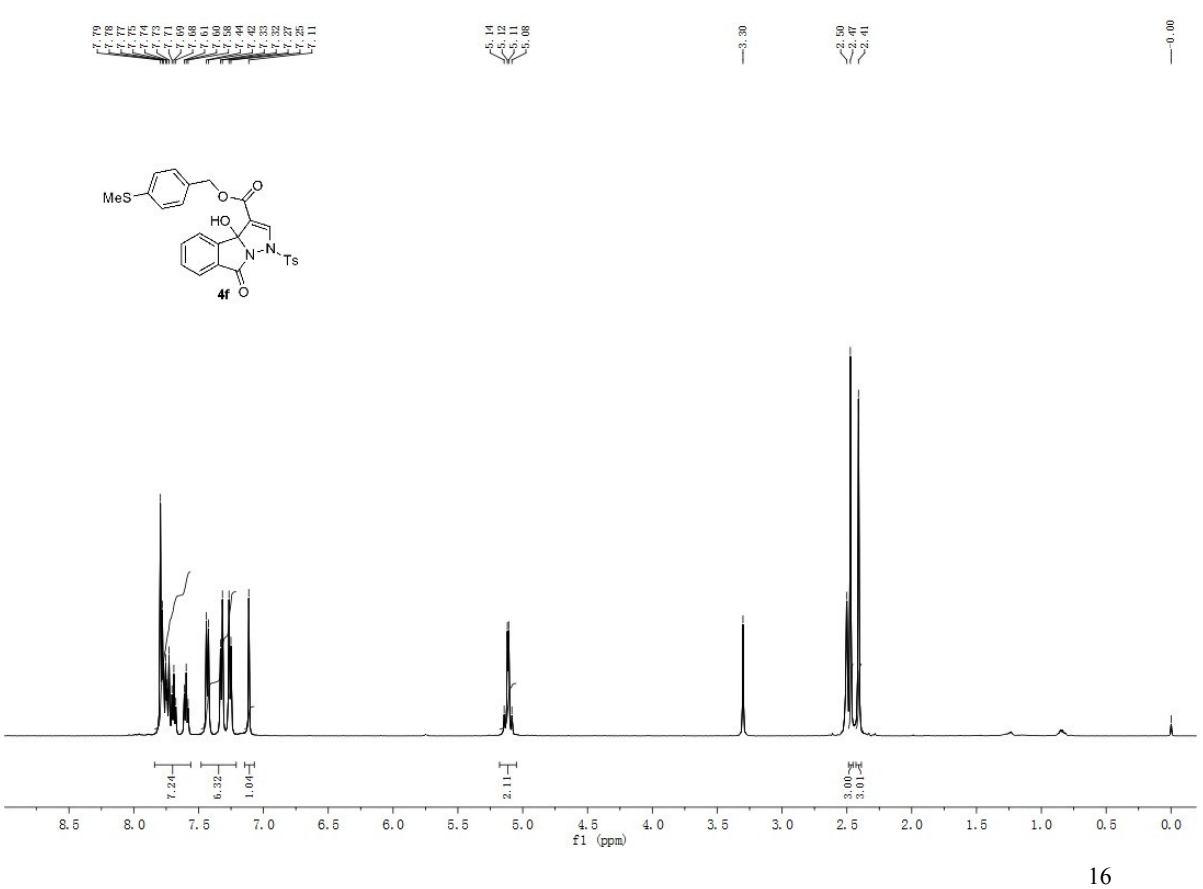
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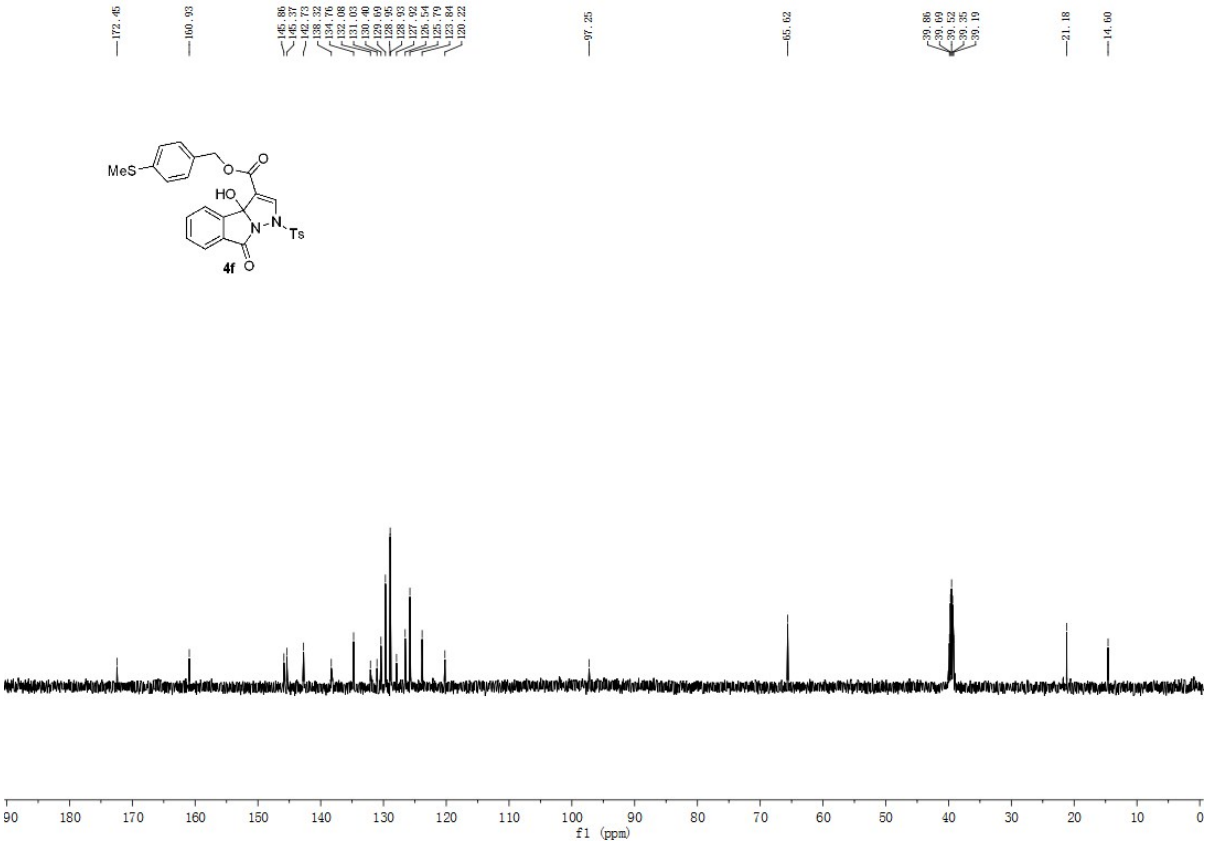
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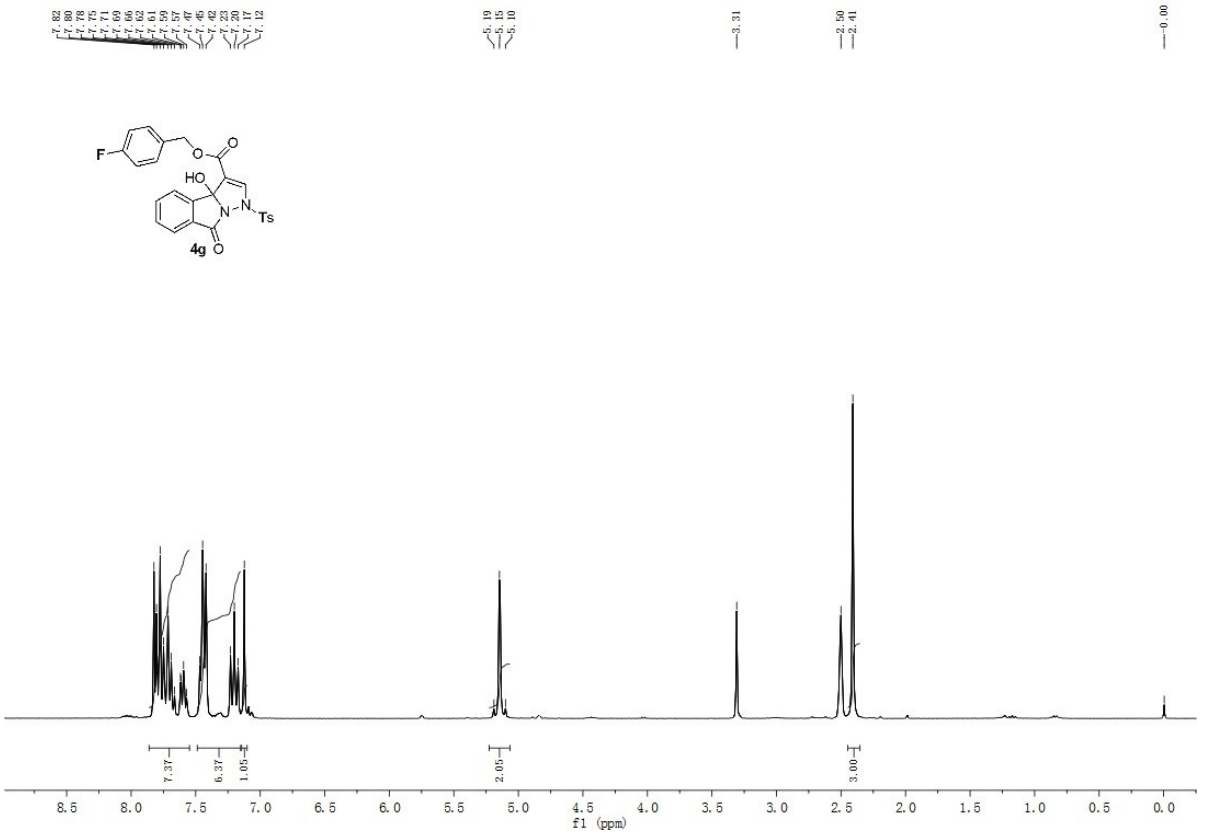
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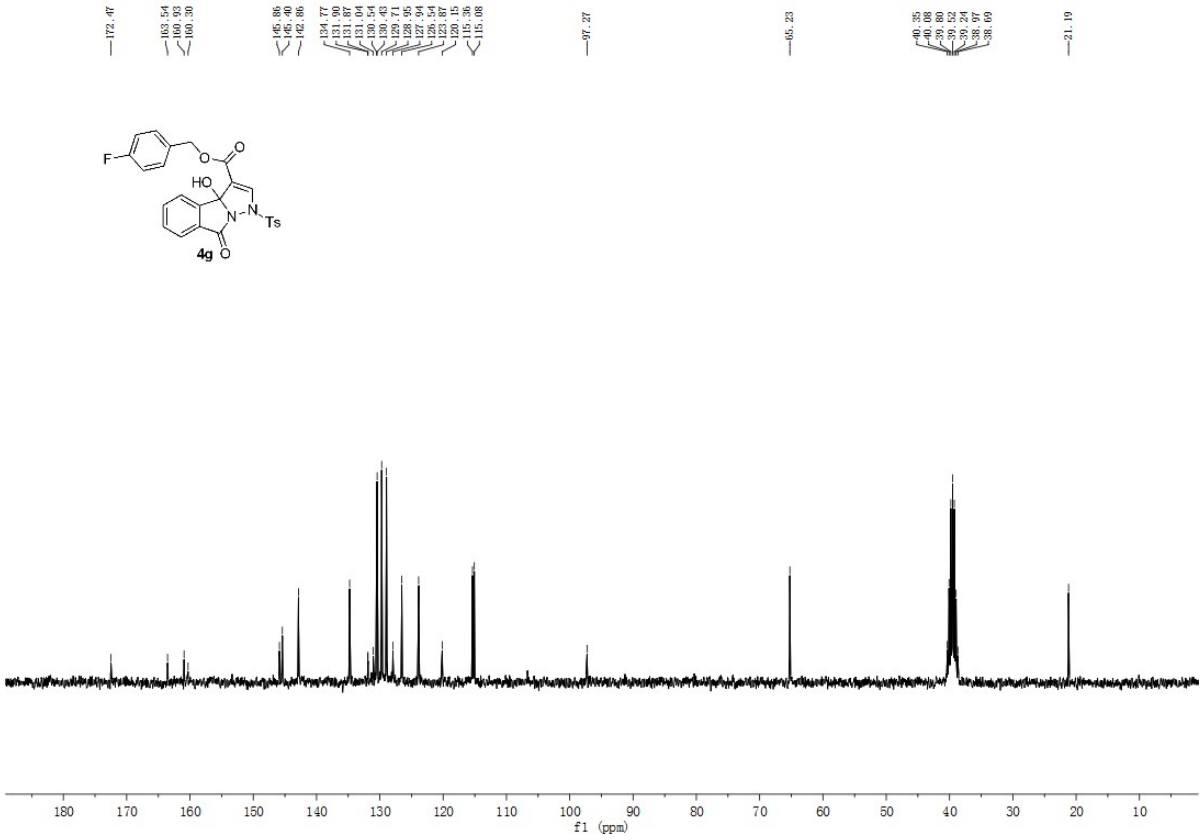
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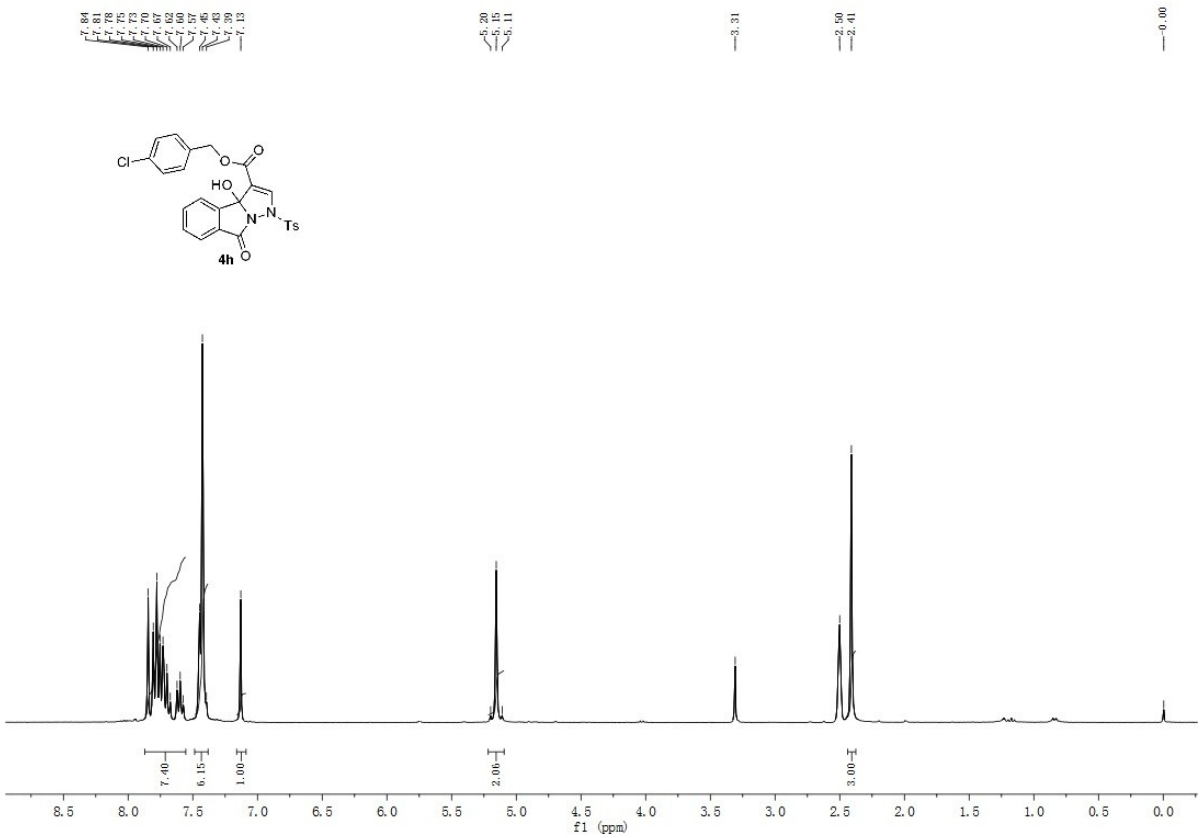
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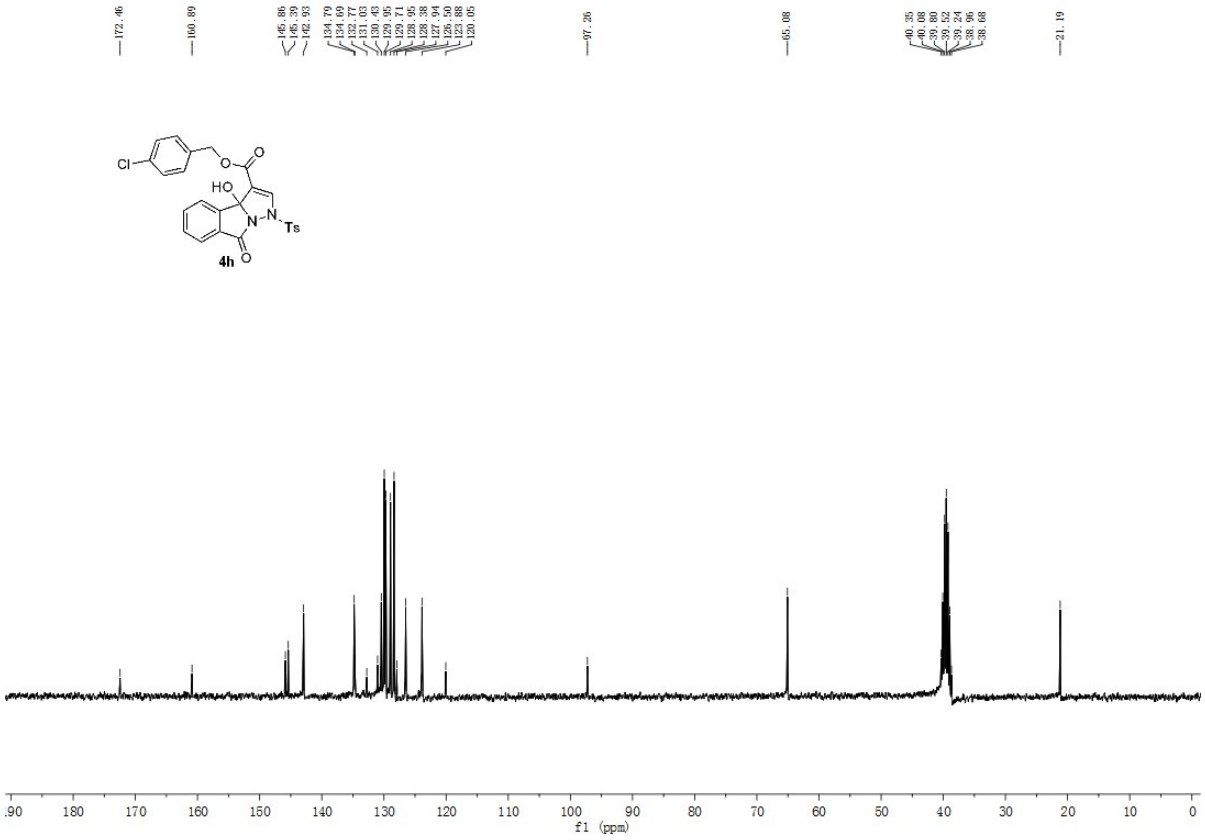
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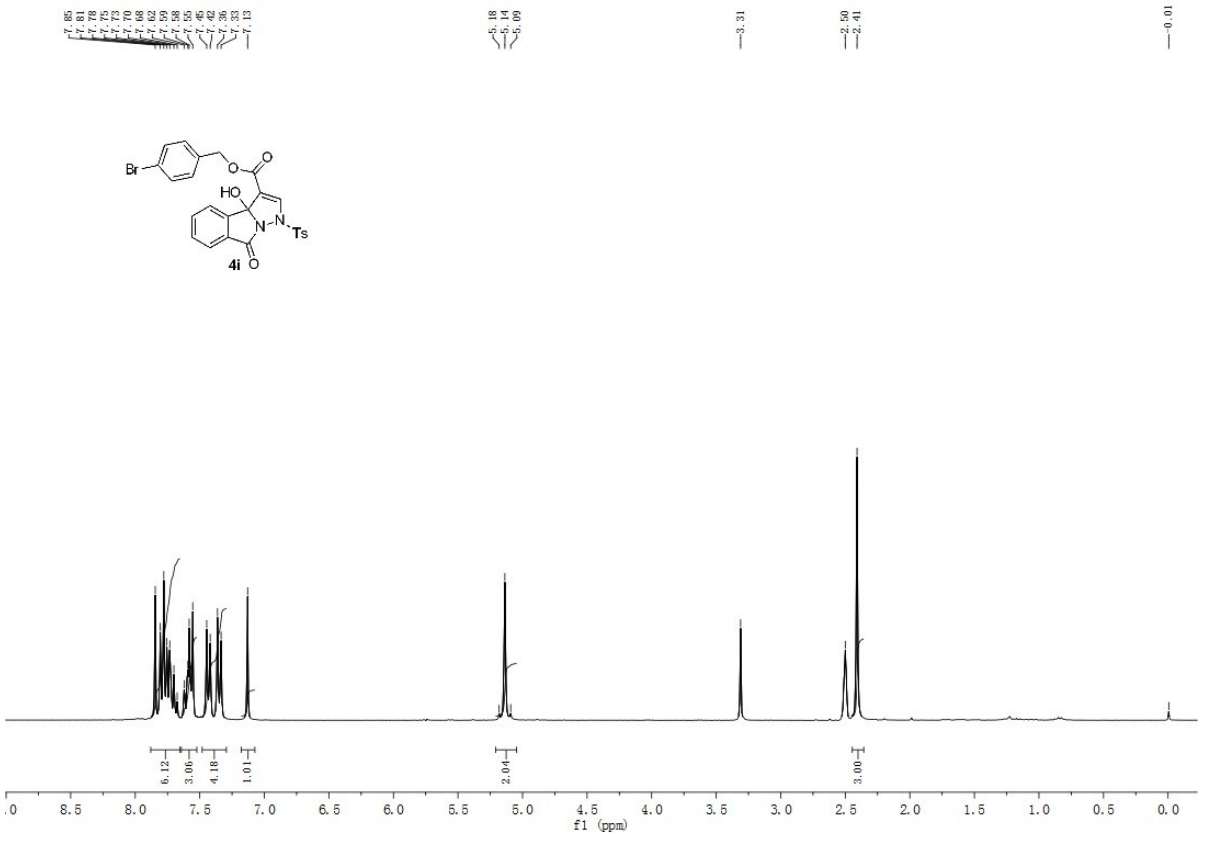
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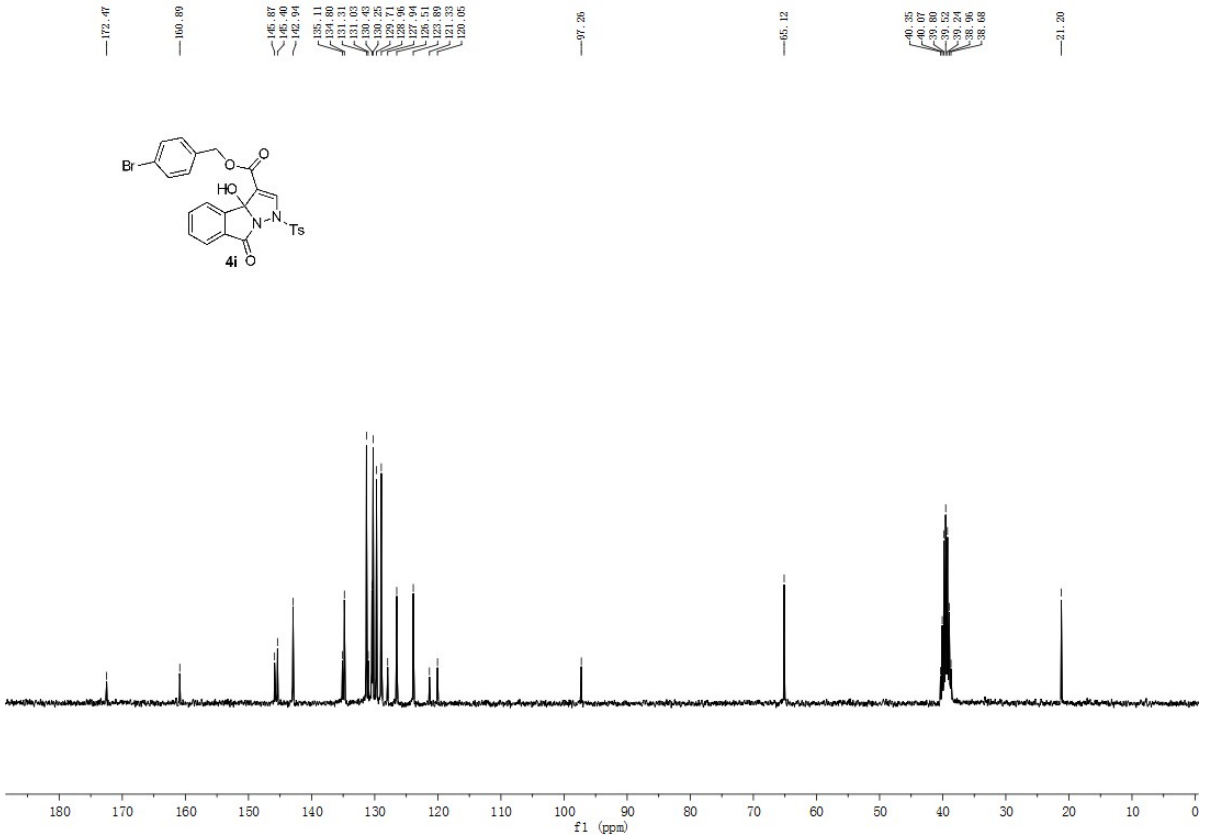
f1 (ppm)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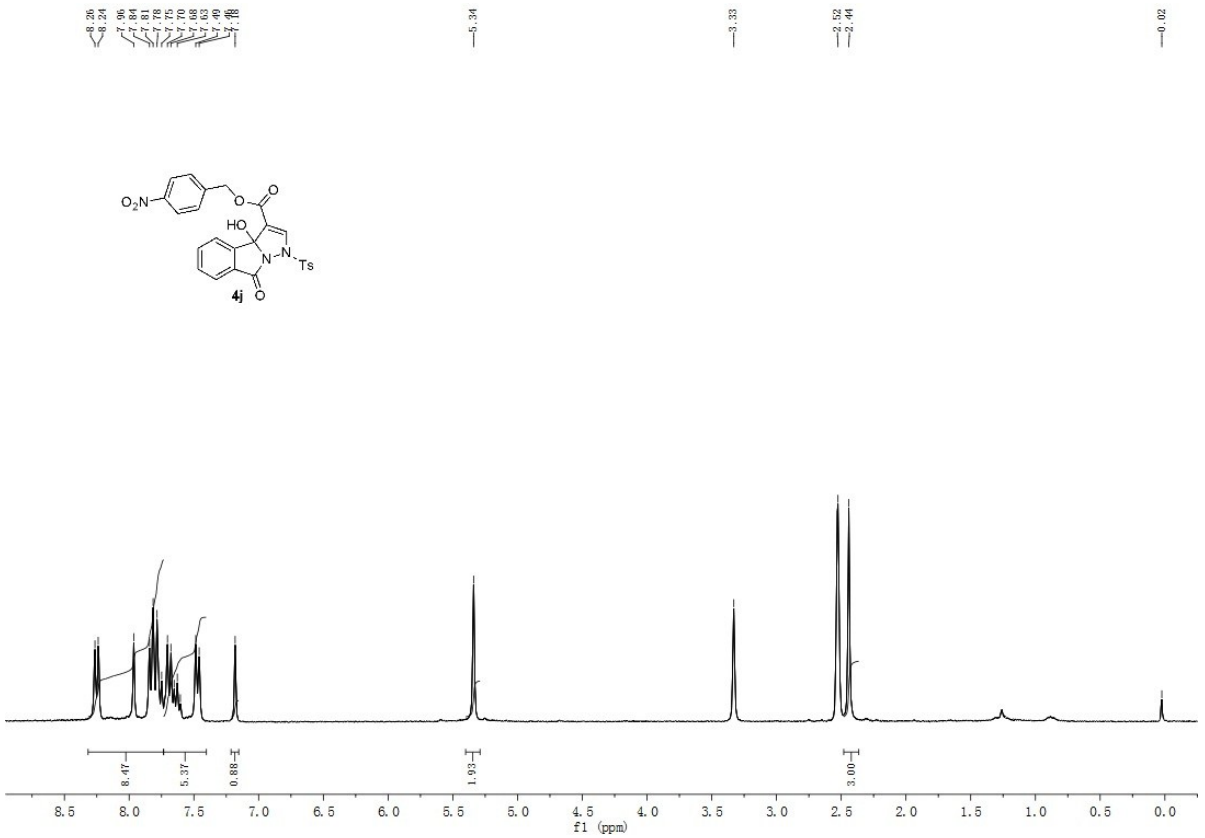
f1 (ppm)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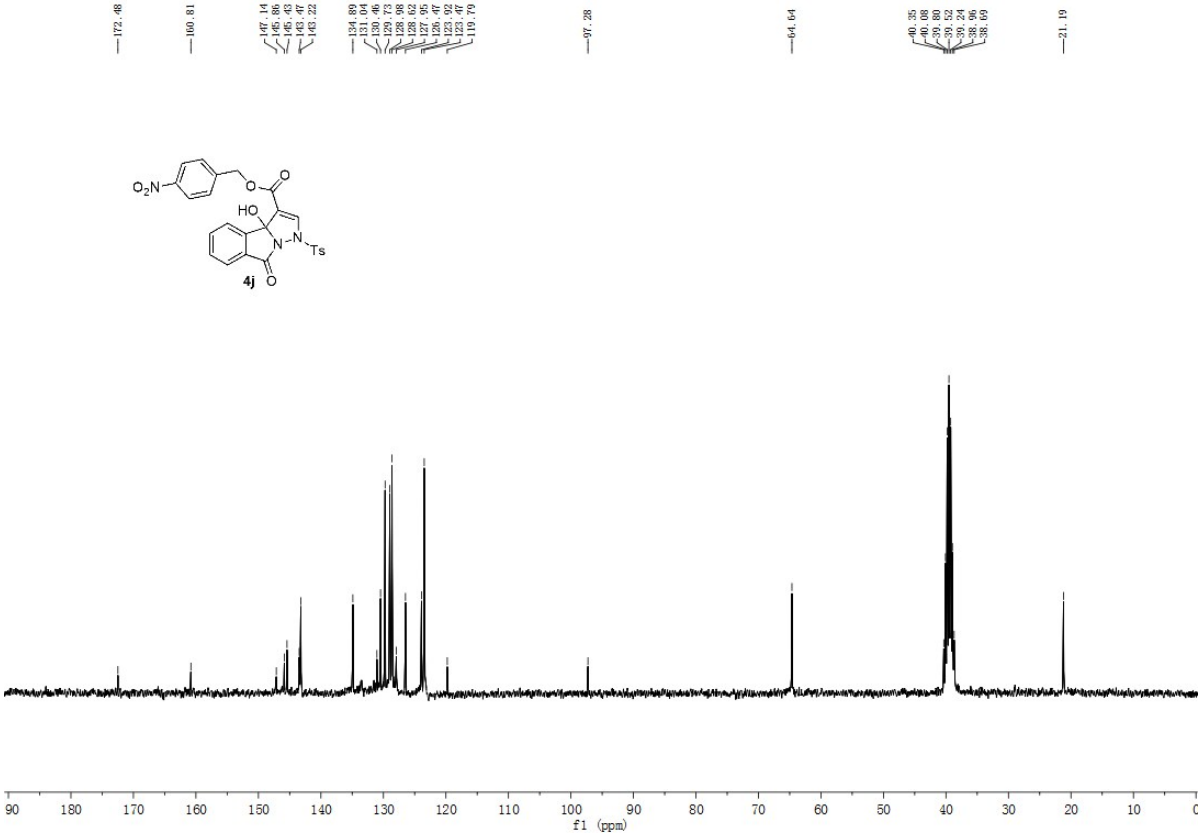
f1 (ppm)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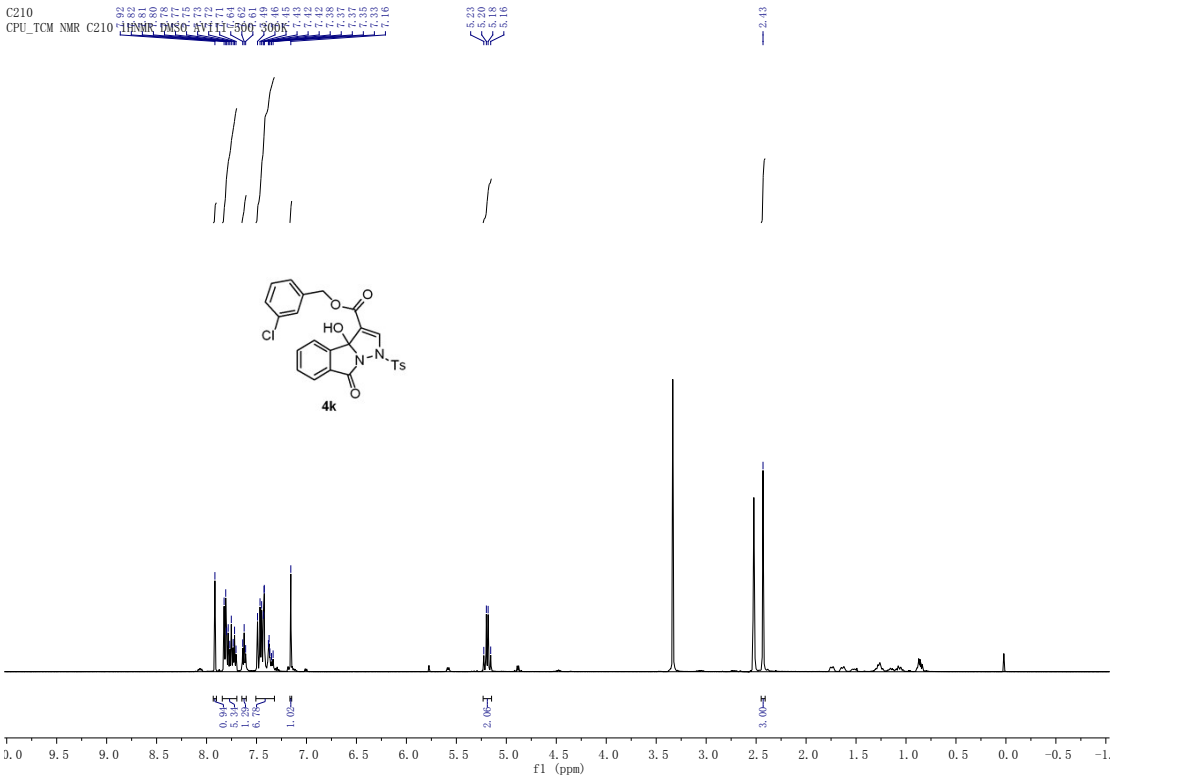
147.14
145.86
145.43
143.47
143.22
134.89
131.04
130.46
129.73
128.98
128.62
127.95
126.47
125.92
123.47
119.79
97.28
64.64
40.35
40.08
39.80
39.52
39.24
38.96
38.69
21.19
O2N
HO
N-N
Ts
O
4j
f1 (ppm)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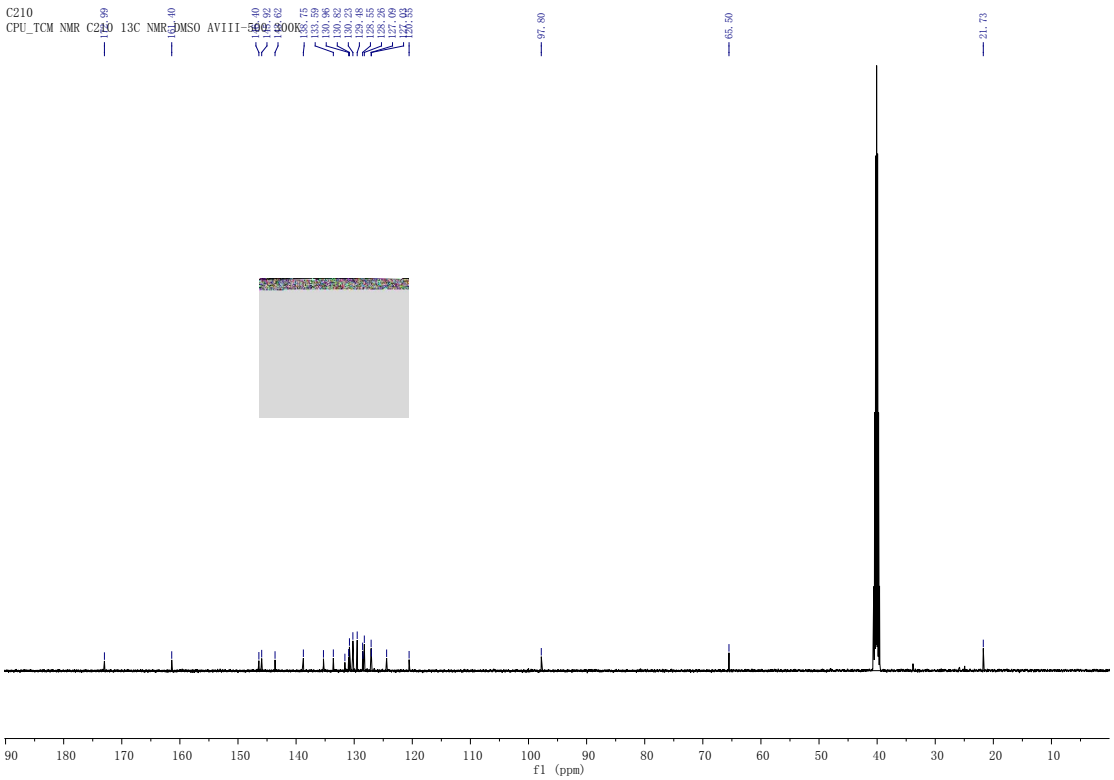
CPU_TCM NMR C210 1HNMR DMSO AVIII-500 2005
7.92
7.82
7.81
7.80
7.78
7.77
7.75
7.73
7.72
7.71
7.64
7.62
7.61
7.46
7.45
7.43
7.42
7.42
7.38
7.37
7.37
7.37
7.35
7.33
7.16
5.23
5.20
5.18
5.16
2.13
Cl
HO
N-N
Ts
O
4k
0.94
5.34
1.00
6.10
1.02
2.00
3.00
f1 (ppm)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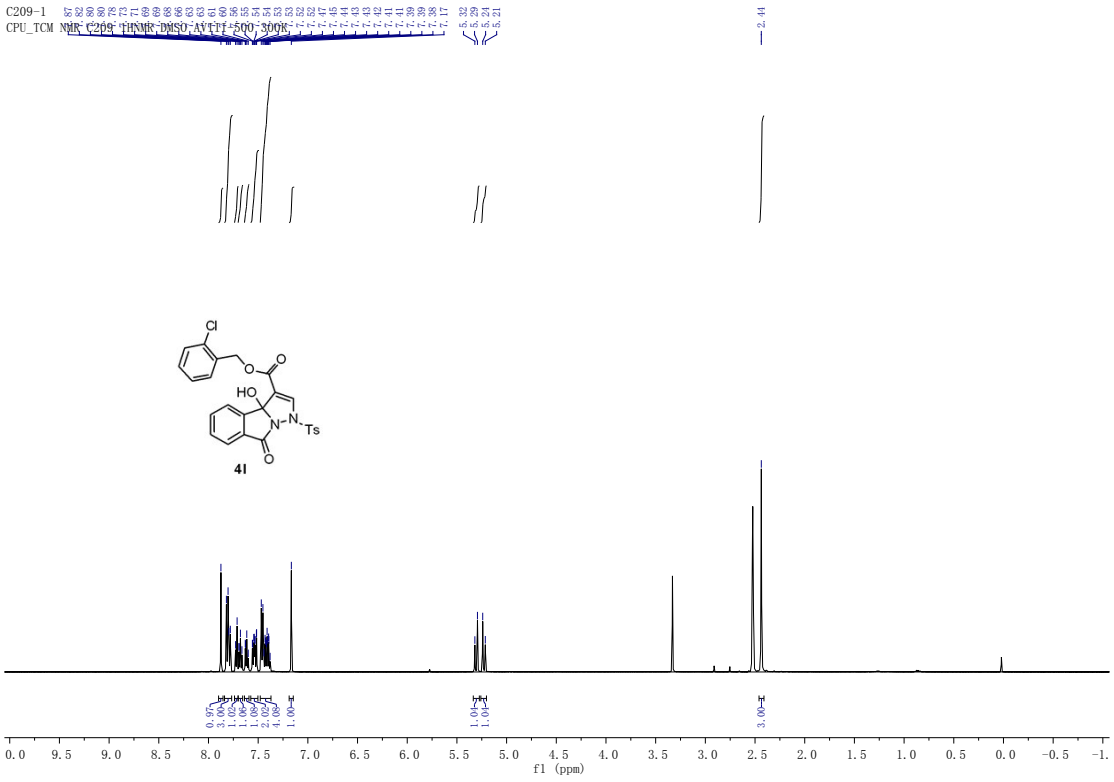
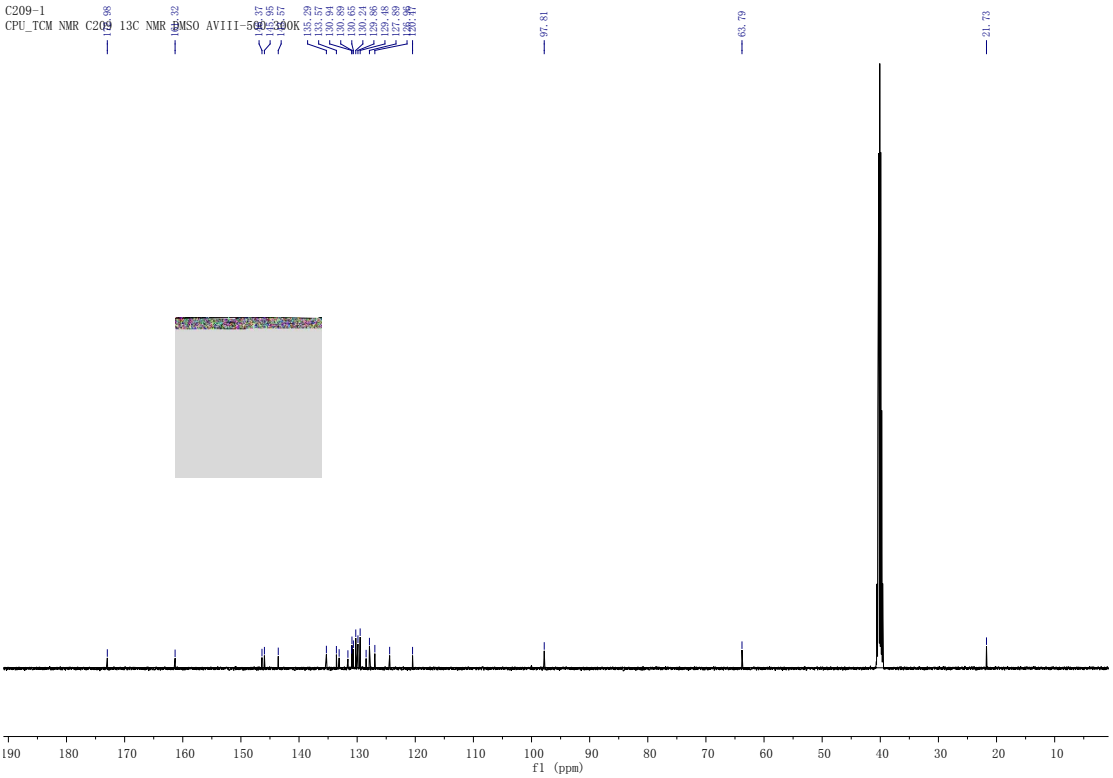
97.80
65.50
21.73
f1 (ppm)


C209-1
CPU_TCM NMR C209-1 1HNMR-DMSO-AVIII-500-300K
2.44
f1 (ppm)


Cl
O
O
HO
N
N
Ts
O

4l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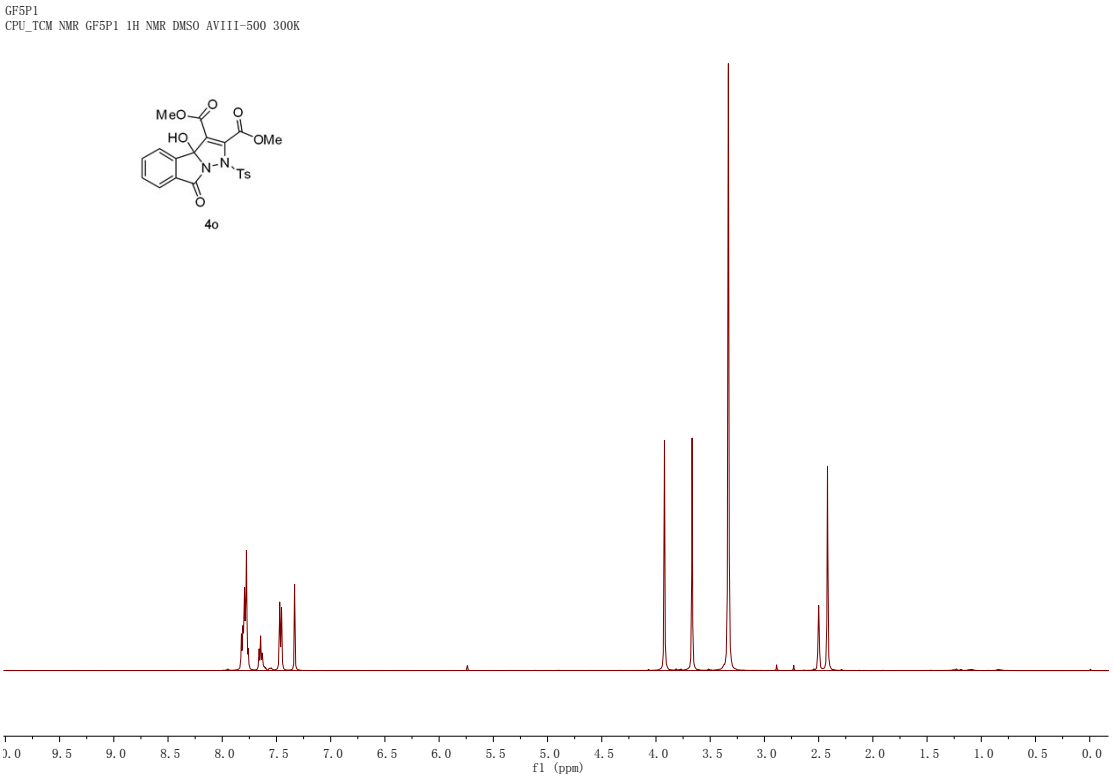
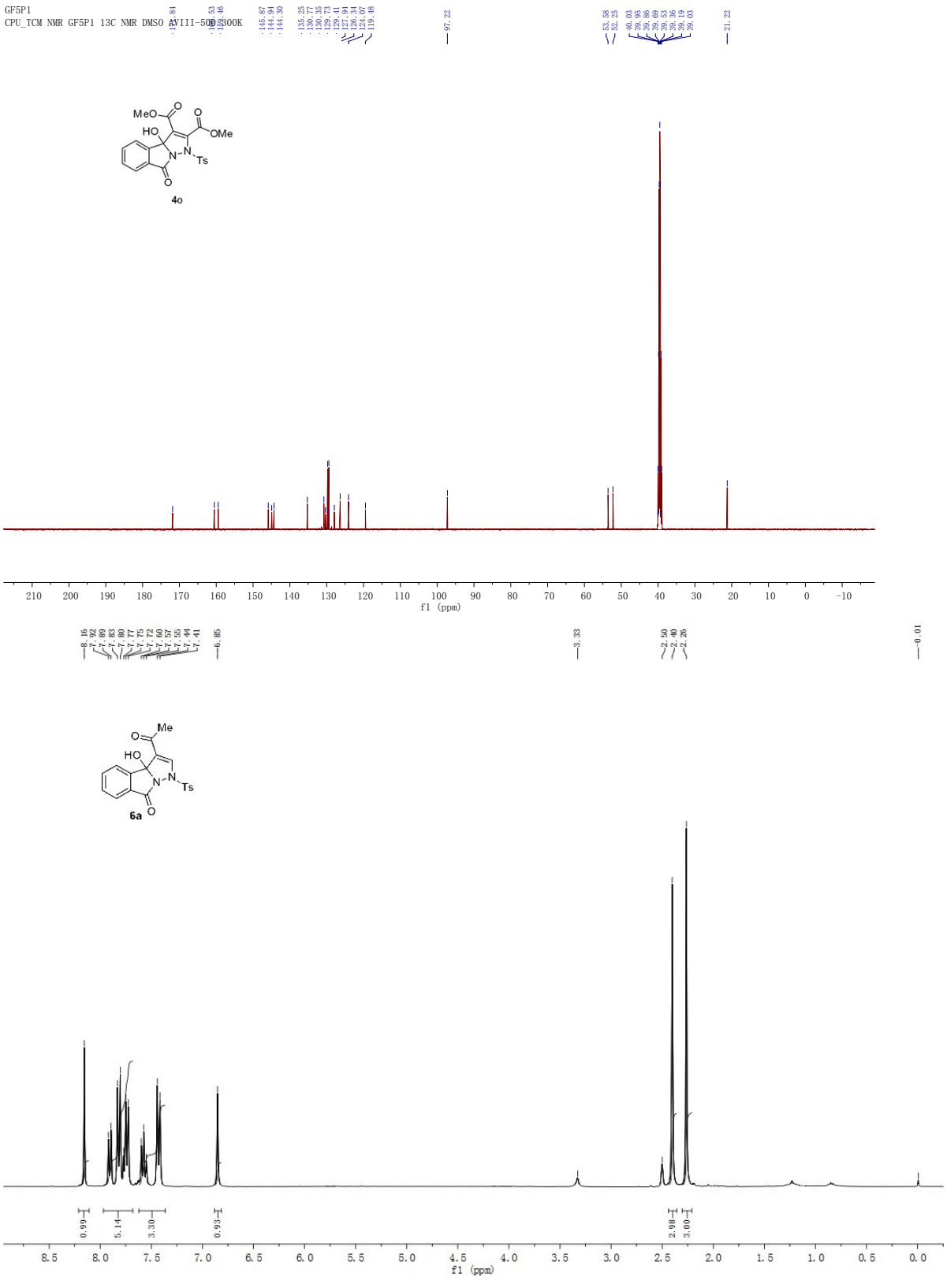
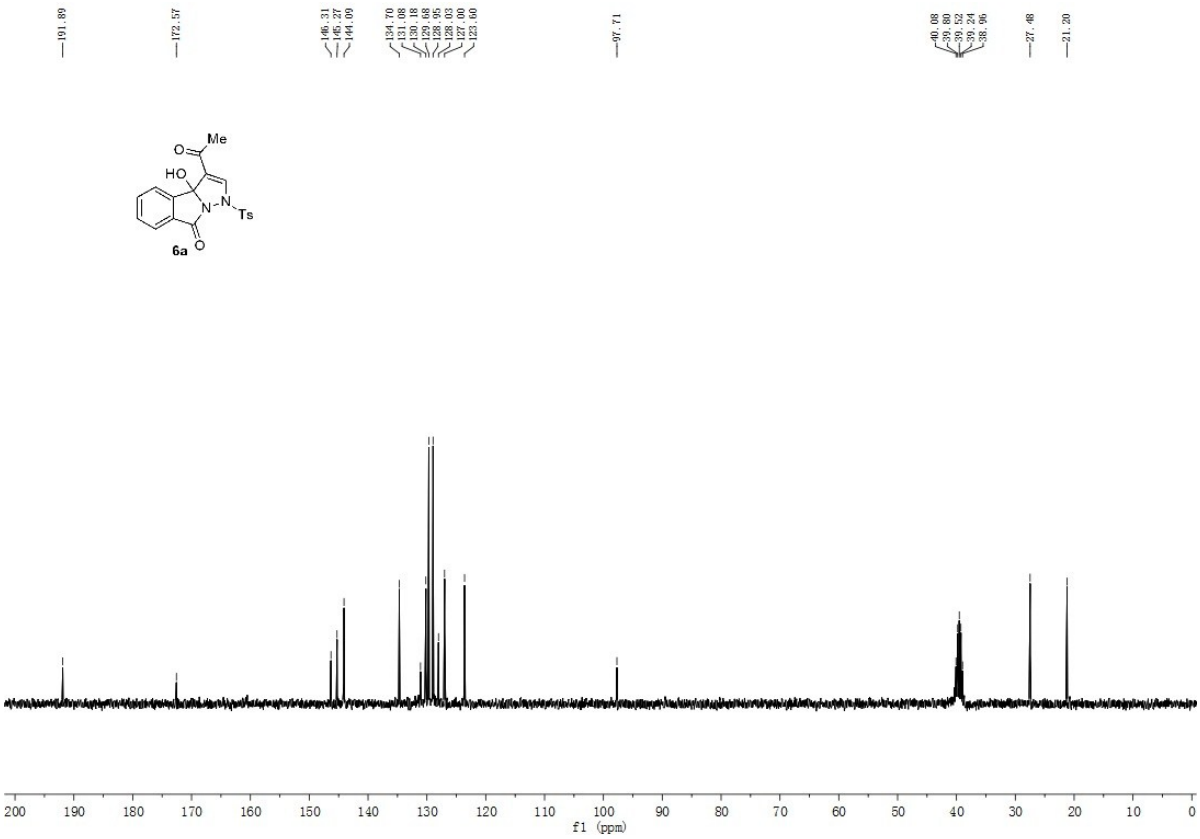
97.81
63.79
21.73
f1 (ppm)


GF5P1
CPU_TCM NMR GF5P1 1H NMR DMSO AVIII-500 300K
MeO
HO
OMe
N
Ts
O
4o
f1 (ppm)


GF5P1
CPU_TCM NMR GF5P1 13C NMR DMSO AVIII-500 BBOOK
MeO
O
HO
OMe
N
Ts
4o
f1 (ppm)
Me
6a
f1 (ppm)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128.95
128.03
127.00
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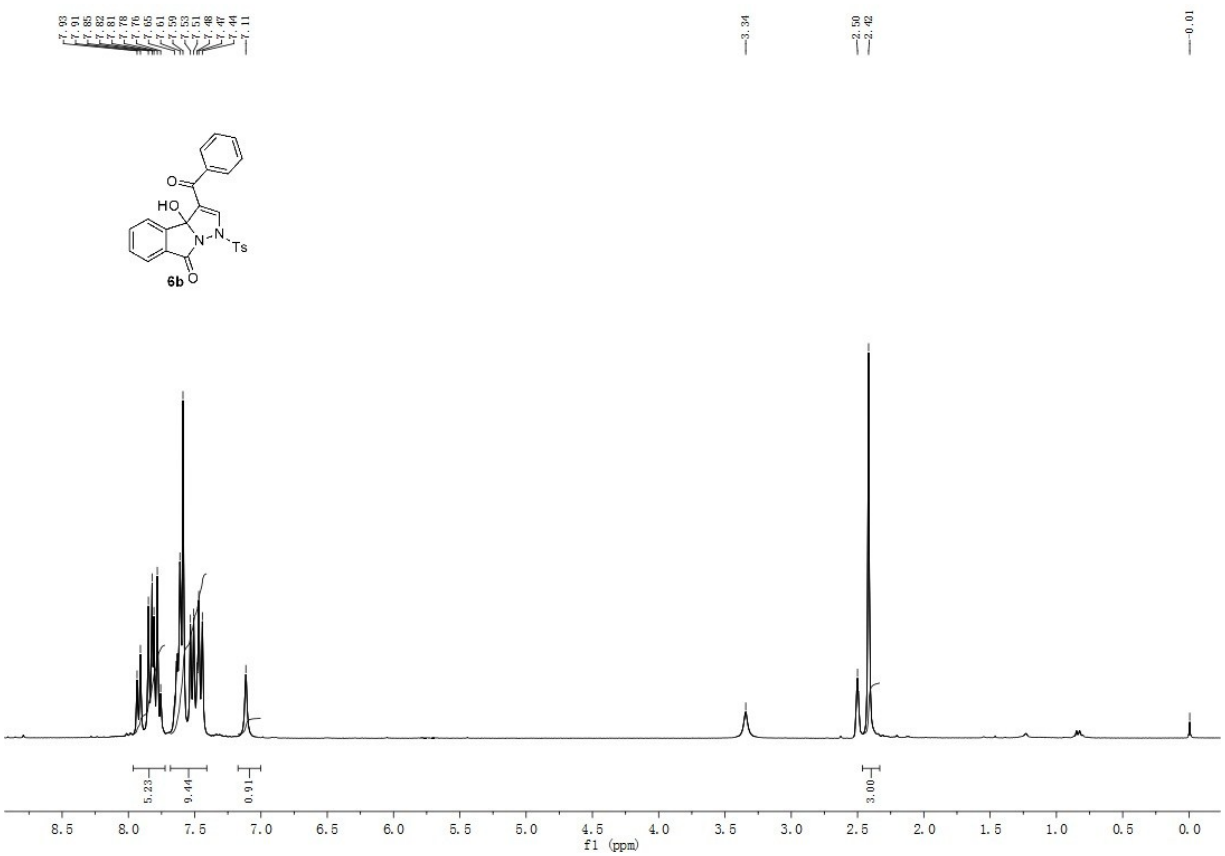
97.71
40.08
39.80
39.52
39.24
38.96
27.48
21.20
Me
O
HO
N
N
Ts
O
6a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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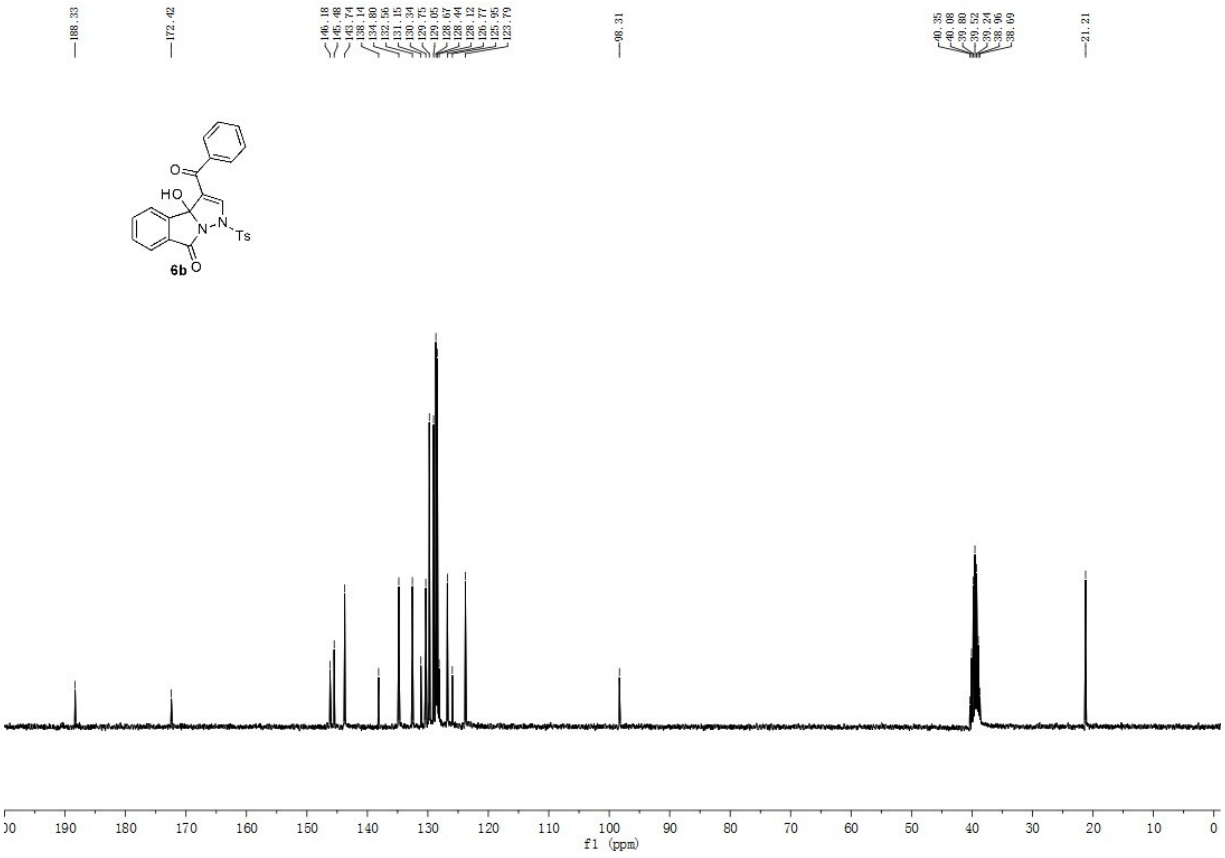
7.91
7.85
7.82
7.81
7.78
7.76
7.65
7.61
7.59
7.53
7.51
7.48
7.47
7.44
7.11
3.34
2.50
2.42
0.01
O
HO
N
N
Ts
O
6b
5.23
9.44
0.91
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


188.33
172.42
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145.48
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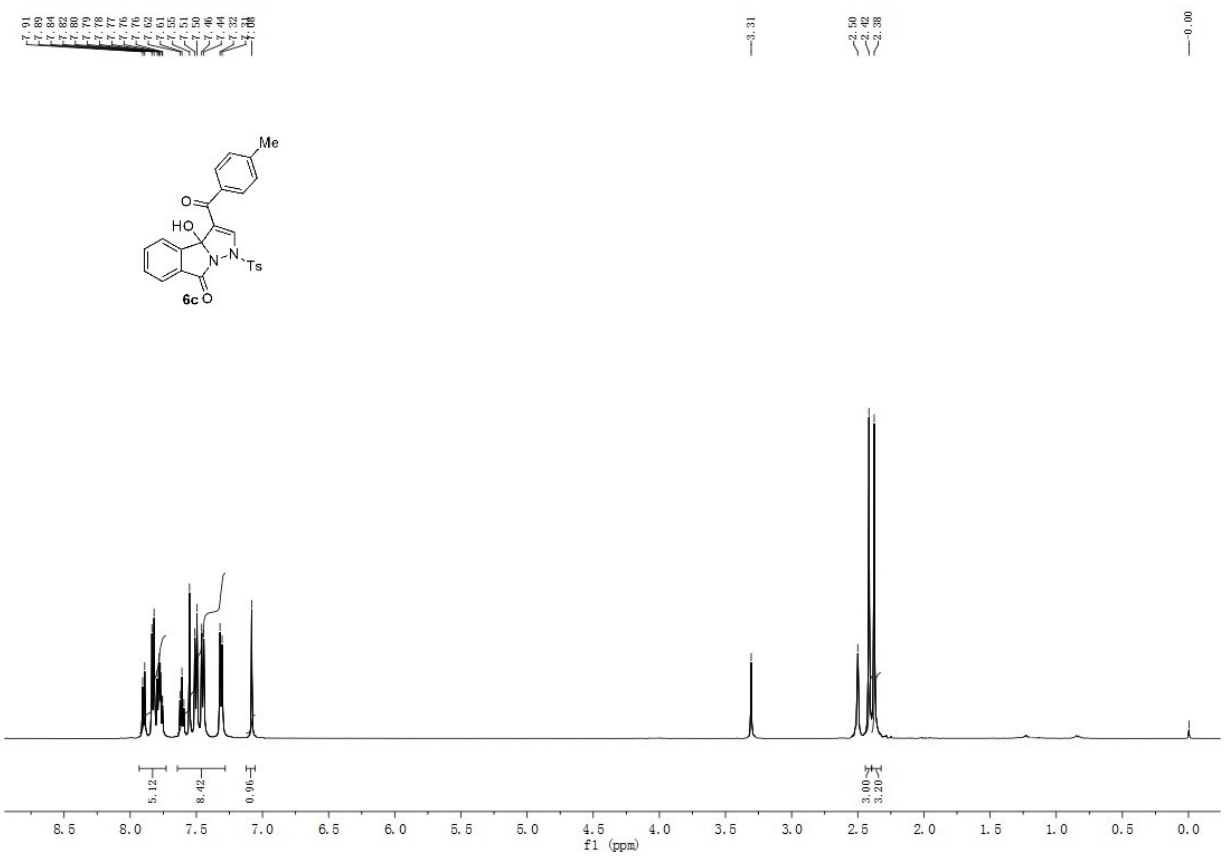
138.14
134.80
132.56
131.15
130.34
129.75
129.05
128.67
128.44
128.12
126.77
125.95
123.79
98.31
40.35
40.08
39.80
39.52
39.24
38.96
38.69
21.21
O
HO
N
N
Ts
O
6b
f1 (ppm)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7.89
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7.82
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7.79
7.78
7.77
7.76
7.76
7.62
7.61
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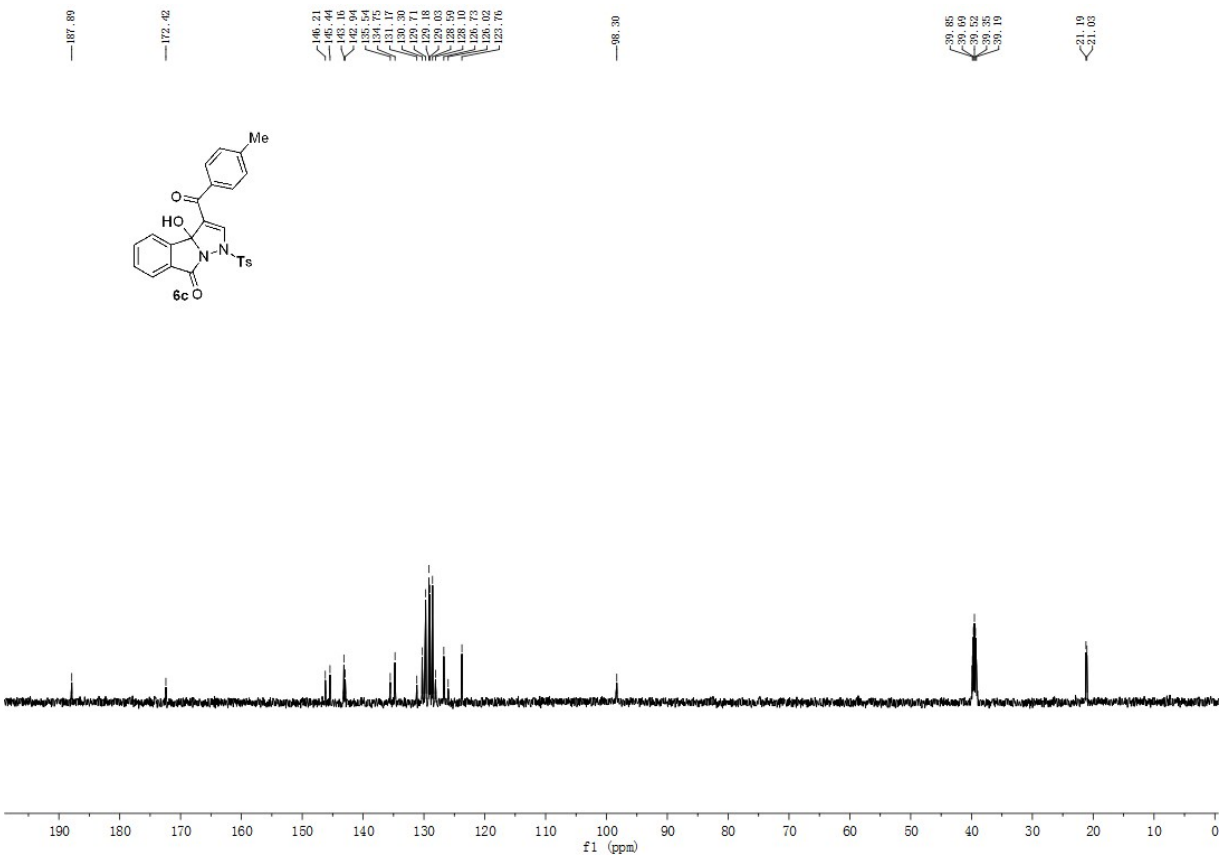
7.51
7.50
7.46
7.44
7.32
7.31
3.31
2.50
2.42
2.38
0.00
Me
O
HO
N
N
Ts
O
6c
5.12
8.42
0.96
3.00
3.20
f1 (ppm)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143.16
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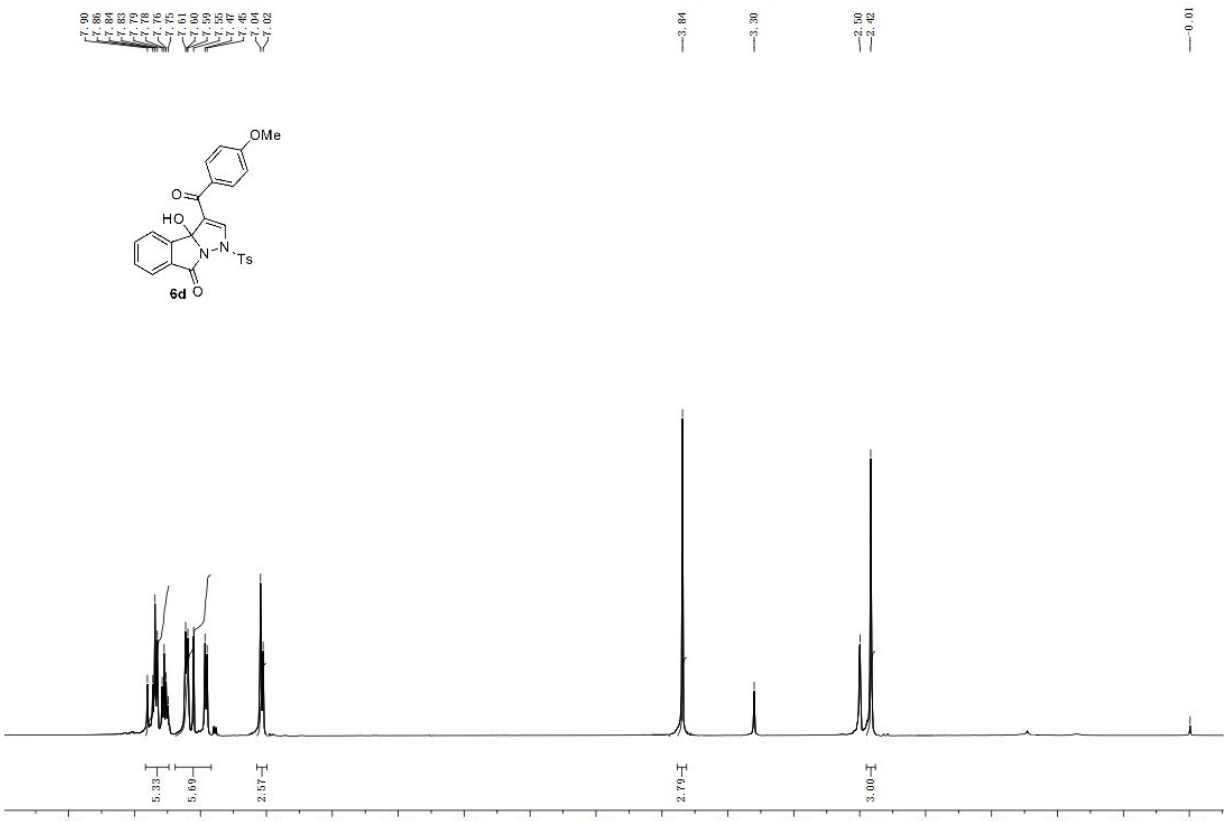
134.75
131.17
130.30
129.71
129.18
129.03
128.93
128.10
126.73
126.02
123.76
98.30
39.85
39.69
39.52
39.35
39.19
21.19
21.03
Me
O
HO
N
N
Ts
O
6c
f1 (ppm)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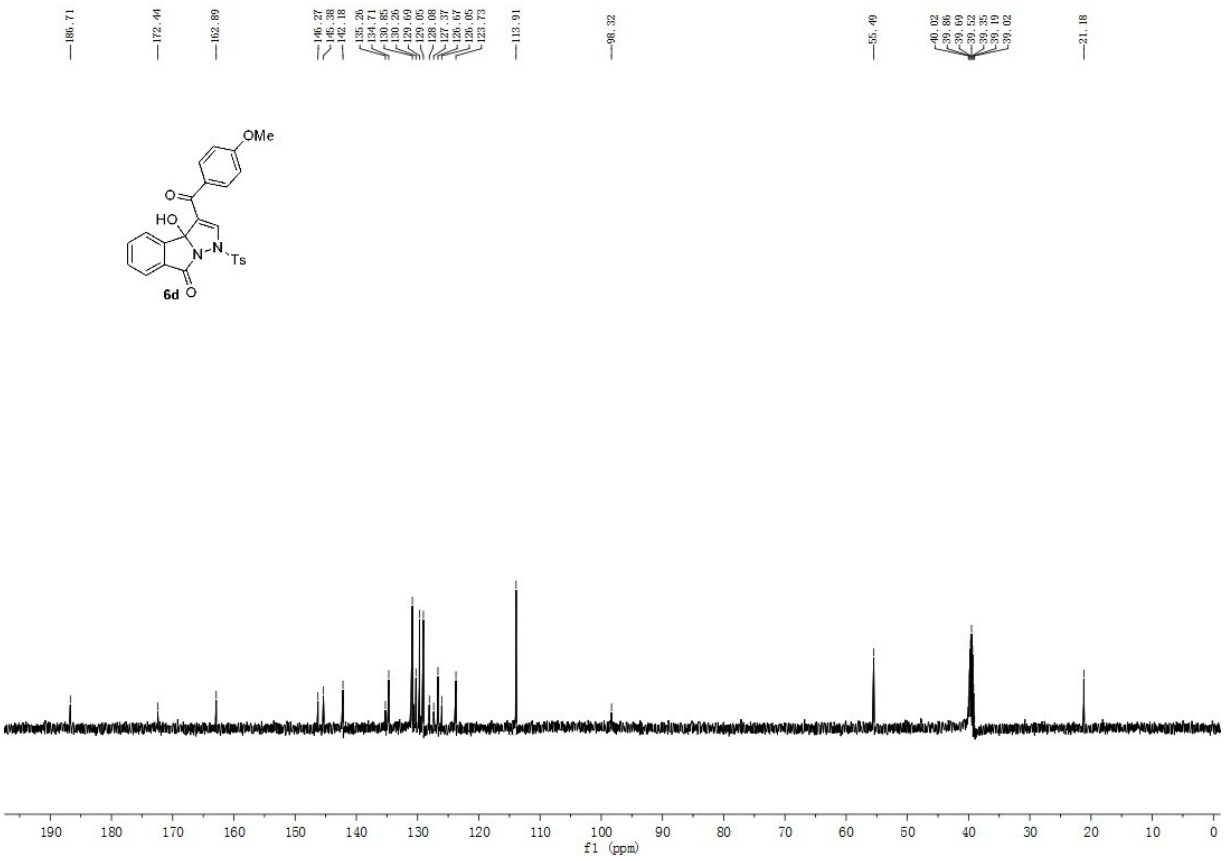
7.86
7.84
7.83
7.79
7.78
7.76
7.75
7.61
7.60
7.59
7.55
7.47
7.04
7.02
3.84
3.30
2.50
2.42
0.01
OMe
O
HO
N
N
Ts
O
6d
5.33
5.69
2.57
2.79
3.00
f1 (ppm)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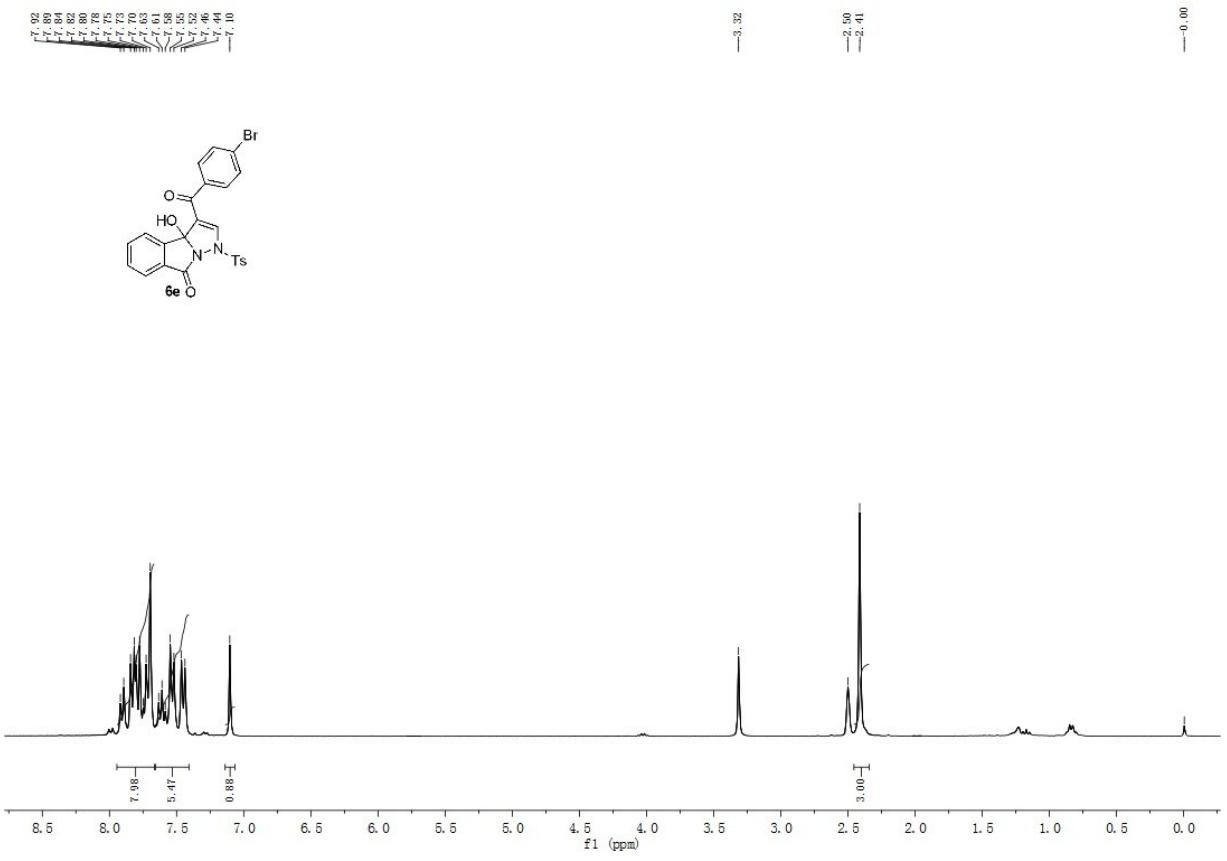
172.44
162.89
146.27
145.38
142.18
135.26
134.71
130.85
130.26
129.69
129.05
128.08
127.37
126.67
126.05
123.73
113.91
98.32
55.49
40.02
39.86
39.69
39.52
39.35
39.19
39.02
21.18
OMe
O
HO
N
N
Ts
O
6d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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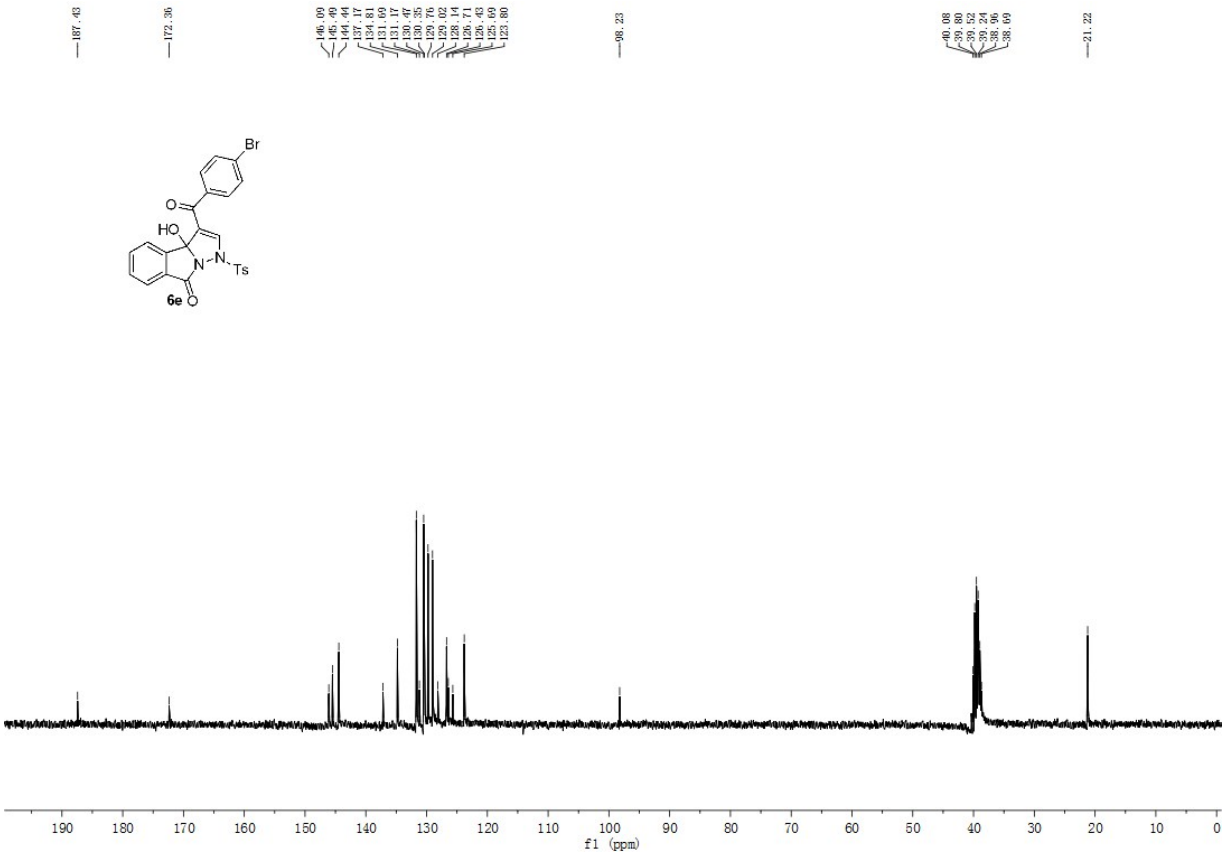
7.89
7.84
7.82
7.80
7.78
7.75
7.73
7.70
7.63
7.61
7.58
7.55
7.52
7.46
7.44
7.10
3.32
2.50
2.41
0.00
Br
O
HO
N
N
Ts
O
6e
7.98
5.47
0.88
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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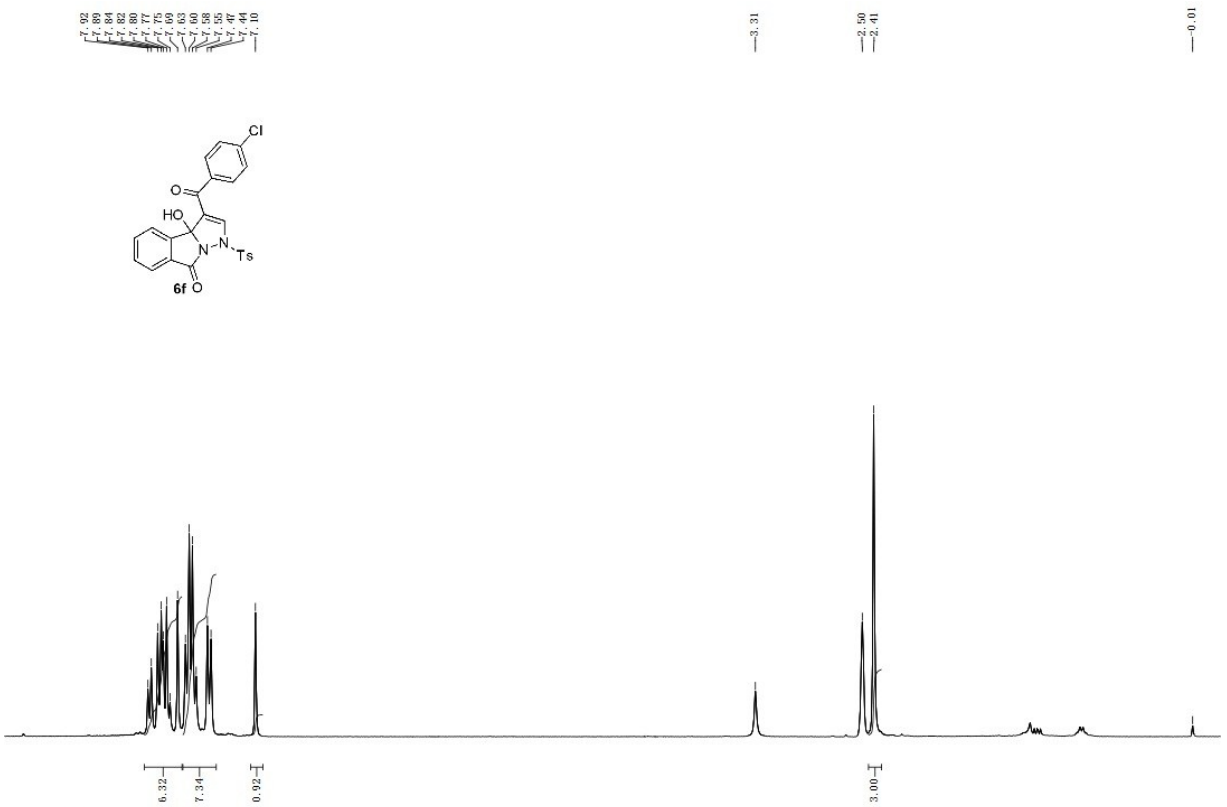
134.81
131.69
131.17
130.47
130.35
129.76
129.02
128.14
126.71
126.43
125.69
125.60
98.23
40.08
39.80
39.52
39.24
38.96
38.69
21.22
Br
O
HO
N
Ts
O
6e
f1 (ppm)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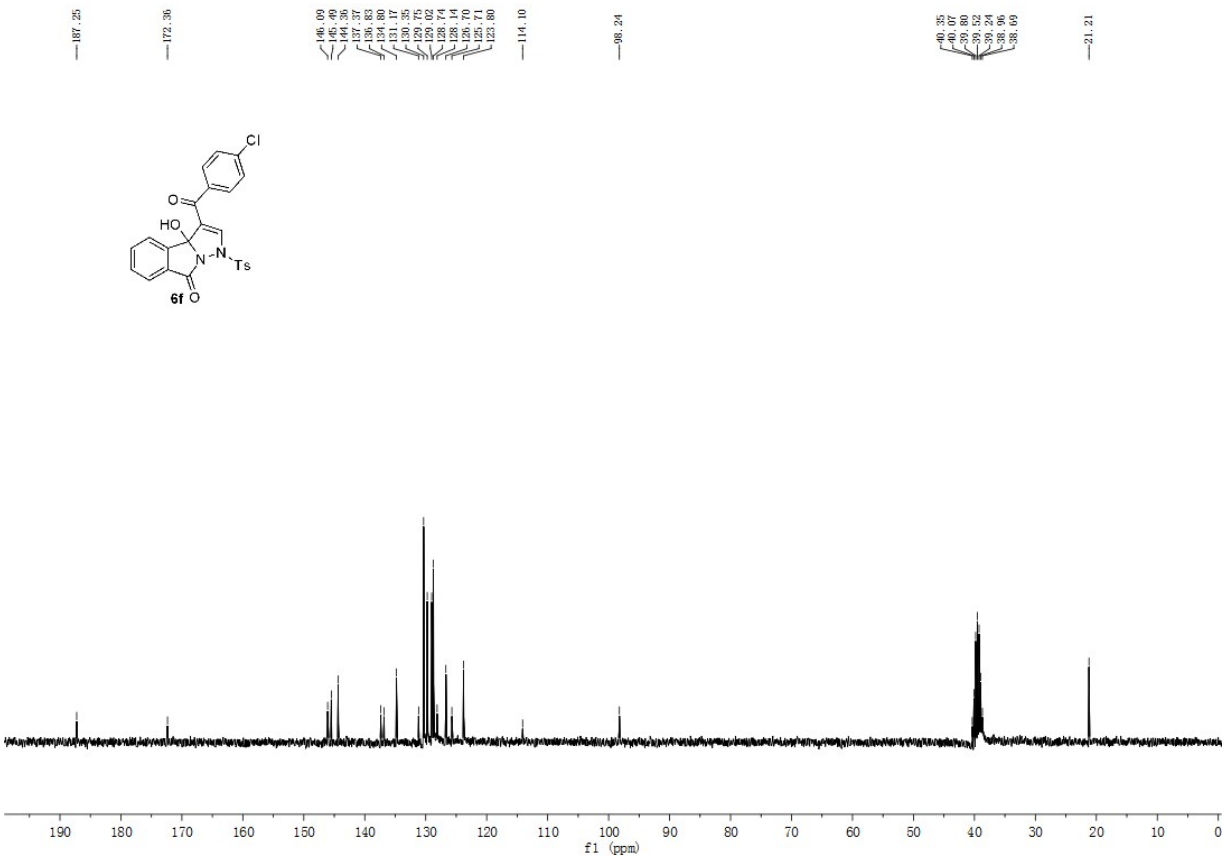
7.89
7.84
7.82
7.80
7.77
7.75
7.69
7.65
7.60
7.58
7.55
7.47
7.44
7.10
3.31
2.50
2.41
0.01
Cl
O
HO
N
Ts
O
6f
6.32
7.34
0.92
3.00
f1 (ppm)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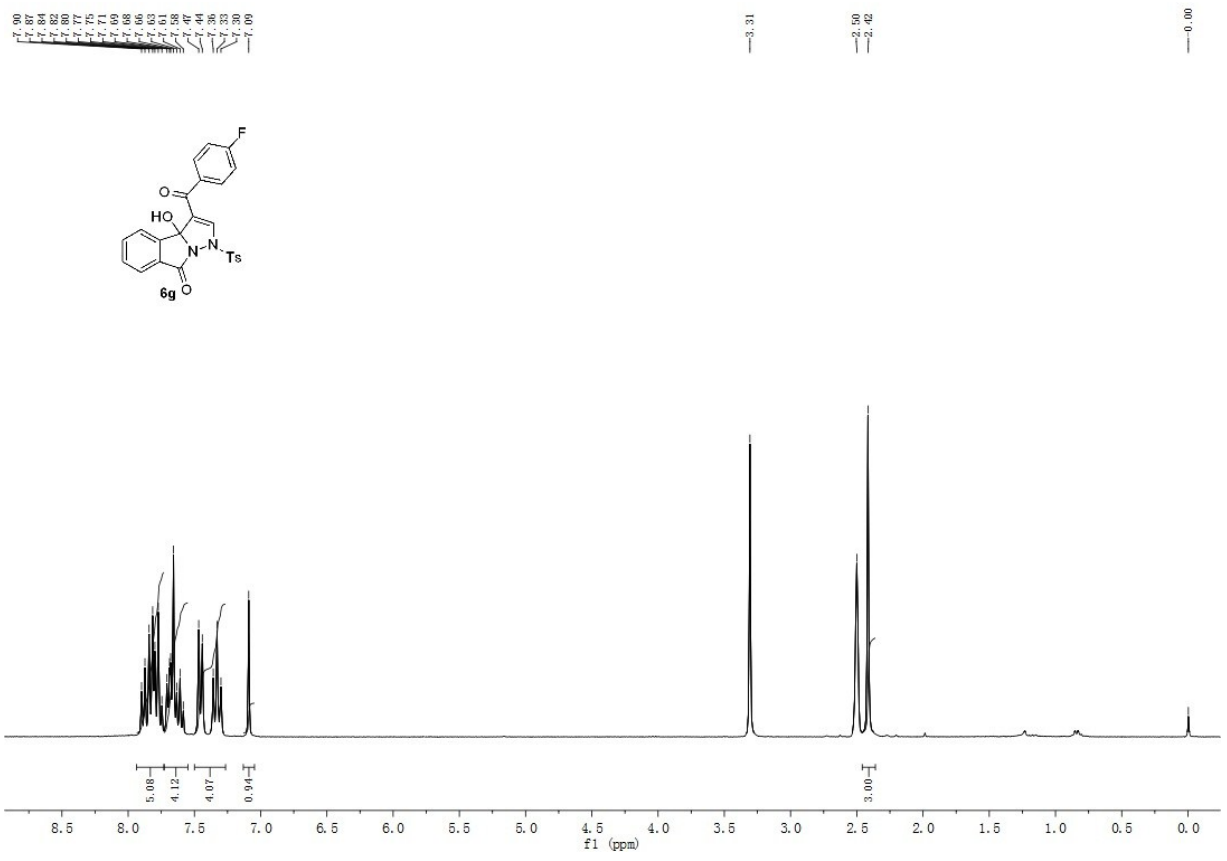
130.35
129.75
129.02
128.74
128.14
126.70
125.71
125.80
114.10
98.24
40.35
40.07
39.80
39.52
39.24
38.96
38.69
21.21
Cl
O
HO
N
N
Ts
O
6f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.71
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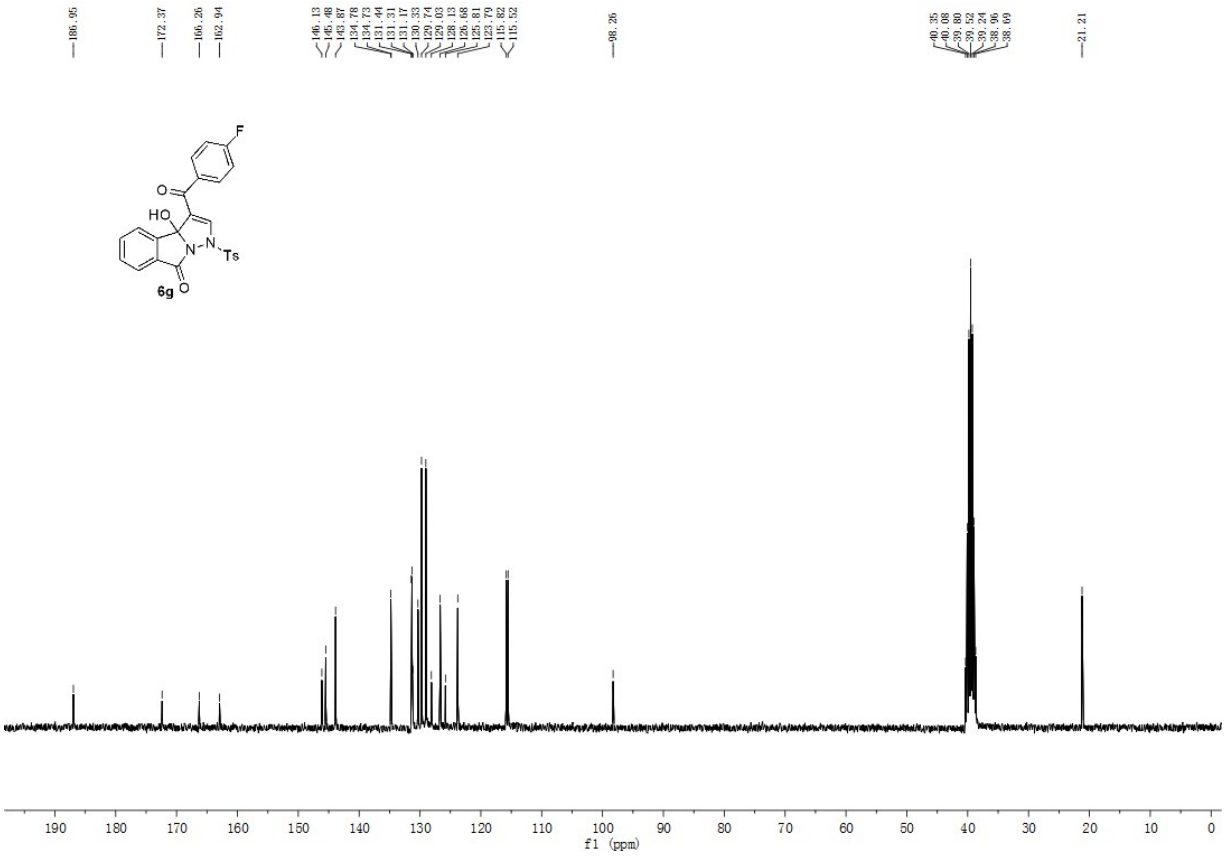
7.68
7.66
7.63
7.61
7.58
7.47
7.44
7.36
7.33
7.30
7.09
3.31
2.50
2.42
0.00
F
O
HO
N
N
Ts
O
6g
5.08
4.12
4.07
0.94
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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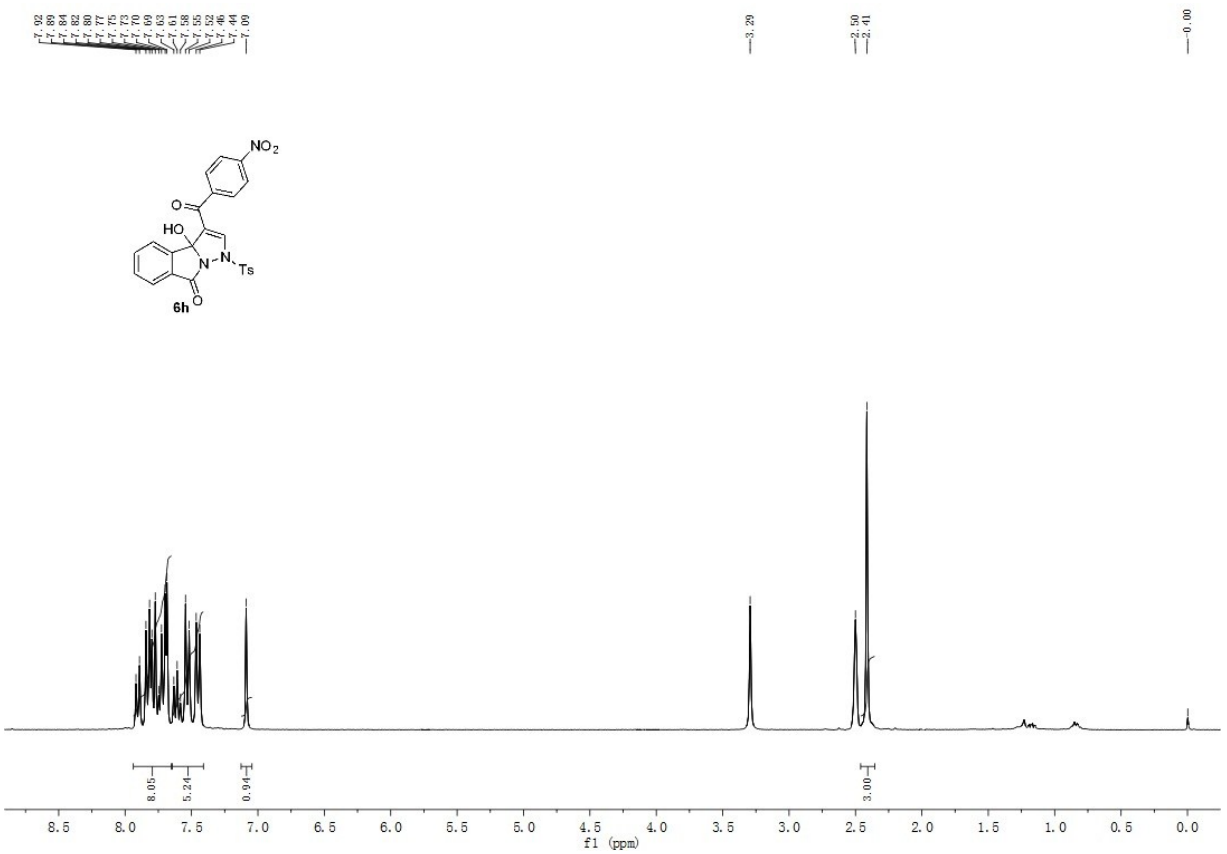
134.73
131.44
131.31
131.17
130.33
129.74
129.03
128.13
126.68
125.81
123.79
115.82
115.52
98.26
40.35
40.08
39.80
39.52
39.24
38.96
38.69
21.21
F
O
HO
N
N
Ts
O
6g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.75
7.73
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7.69
7.63
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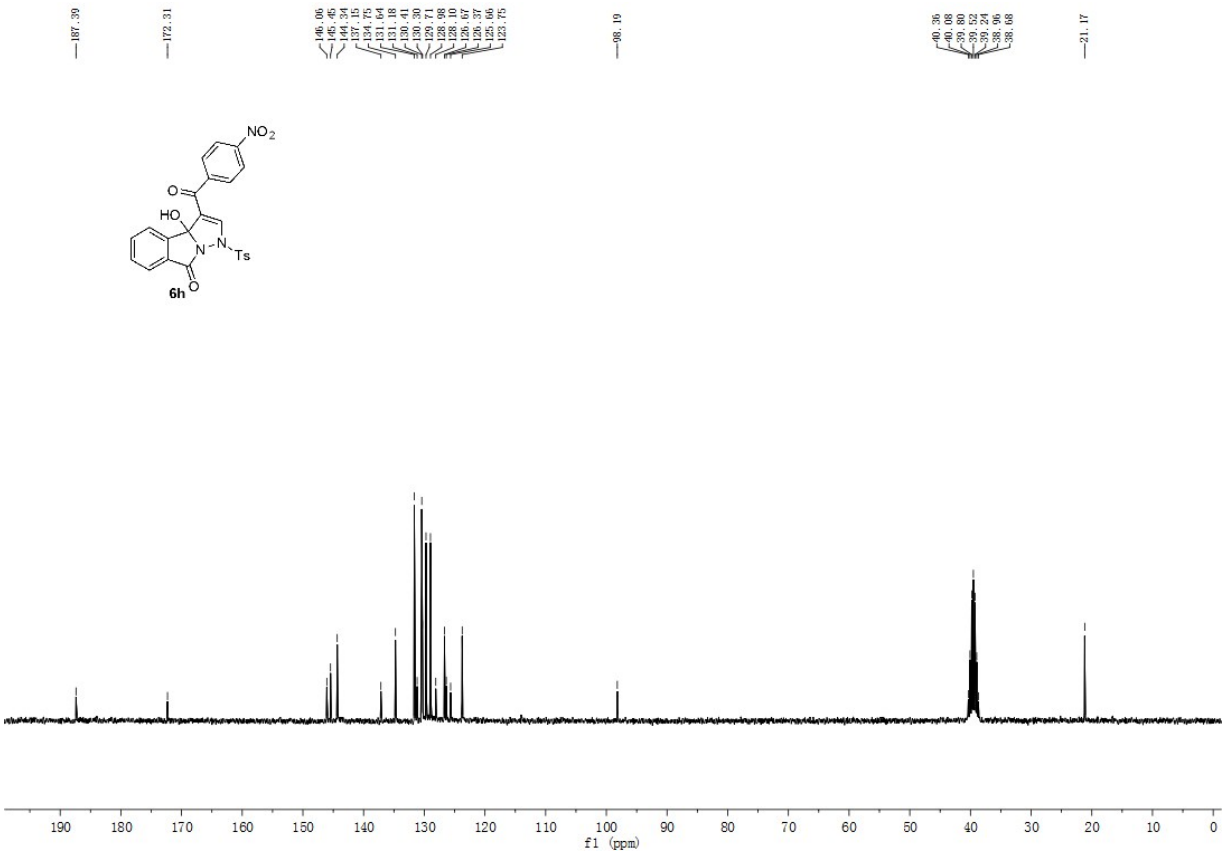
7.58
7.55
7.52
7.46
7.44
7.09
3.29
2.50
2.41
0.00
NO2
O
HO
N
N
Ts
O
6h
8.05
5.24
0.94
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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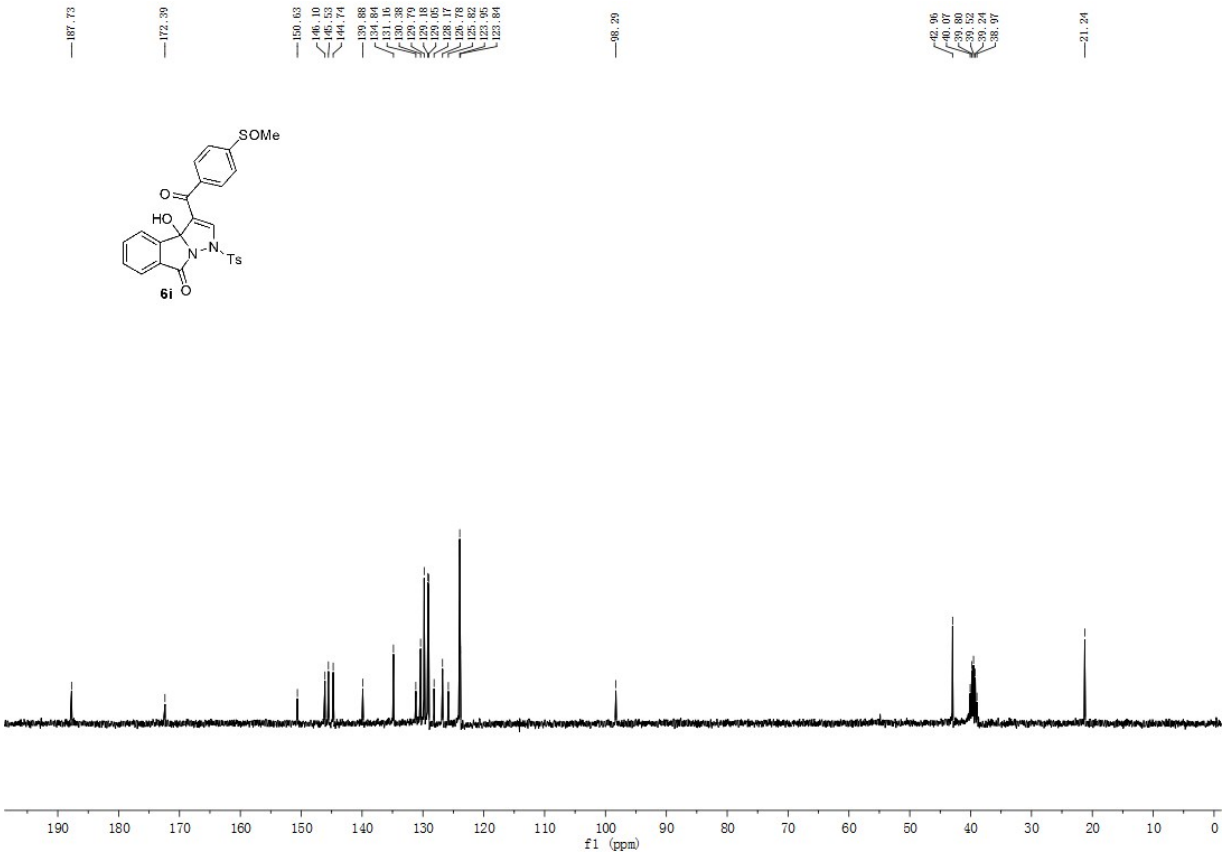
131.64
131.18
130.41
130.30
129.71
128.98
128.10
126.67
126.37
125.66
123.75
98.19
40.36
40.08
39.80
39.52
39.24
38.96
38.68
21.17
NO2
O
HO
N
N
Ts
O
6h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.96
7.93
7.86
7.83
7.81
7.80
7.78
7.76
7.72
7.64
7.61
7.59
7.47
7.44
7.13
2.81
2.50
2.41
0.01
SOMe
O
HO
N
N
Ts
O
6i
9.24
4.07
0.71
2.99
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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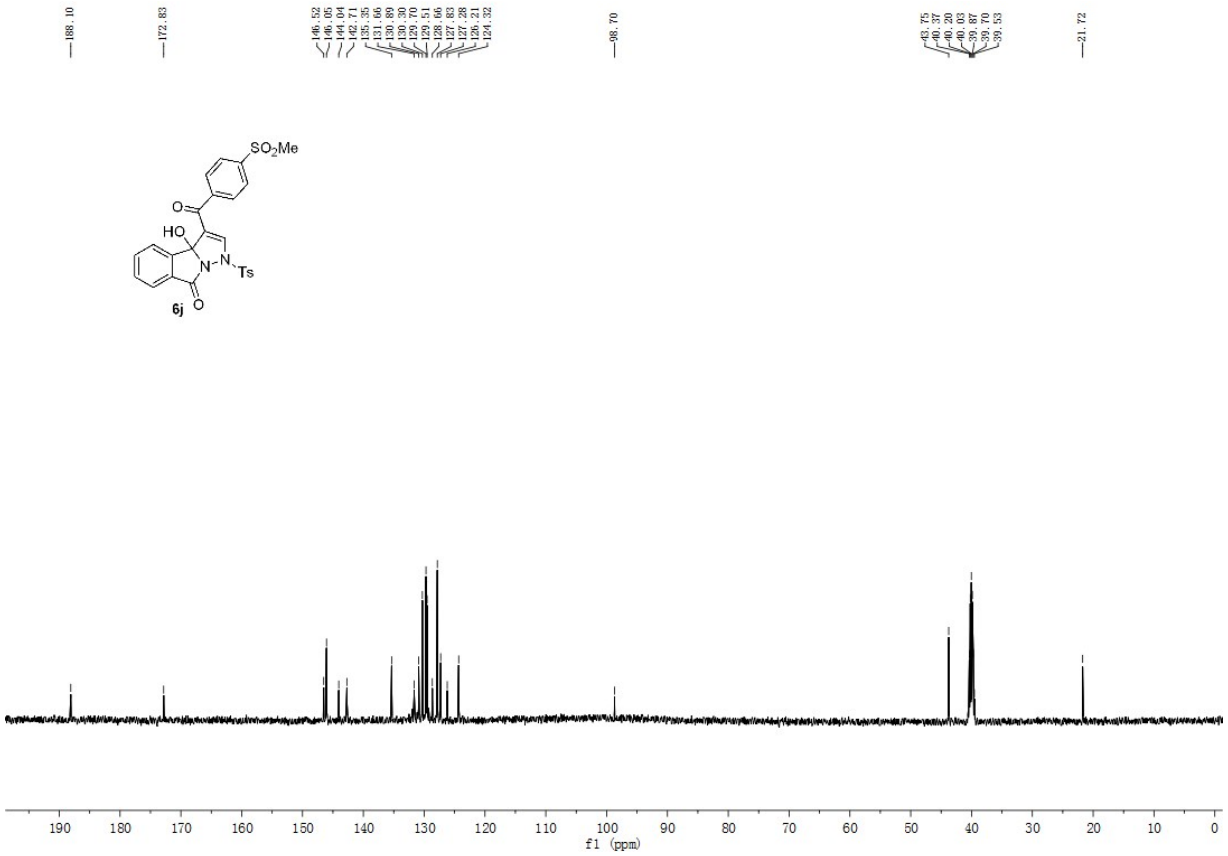
130.38
129.79
129.18
128.95
128.17
126.78
125.82
123.95
123.84
98.29
42.96
40.07
39.80
39.52
39.24
38.97
21.24
SOMe
O
HO
N
N
Ts
O
6i
f1 (ppm)


8.06
8.04
7.96
7.94
7.84
7.83
7.82
7.81
7.79
7.74
7.64
7.62
7.61
7.47
7.45
7.14
3.32
3.28
2.50
2.42
0.00
SO2Me
O
HO
N
N
Ts
O
6j
9.41
4.96
0.93
2.96
3.00
f1 (ppm)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131.66
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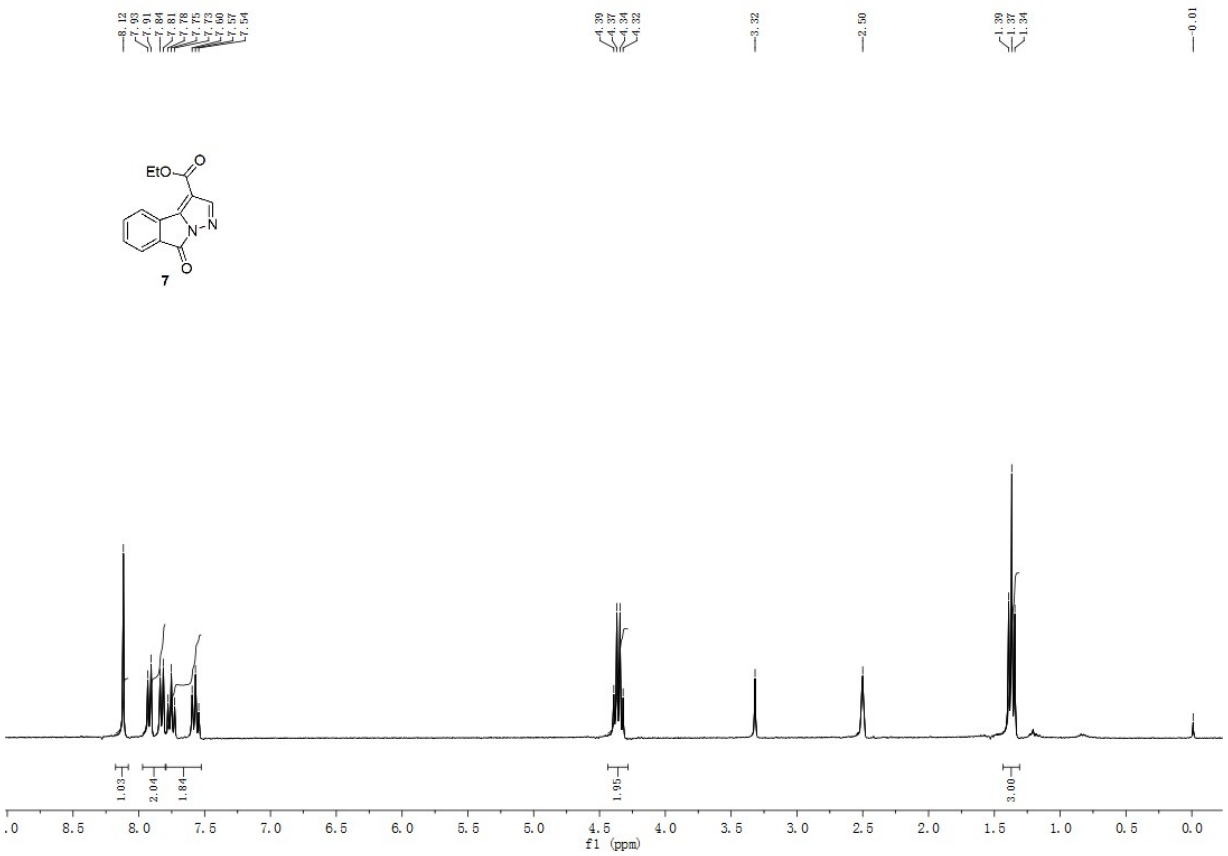
130.30
129.70
129.51
128.66
127.85
127.38
126.21
124.32
98.70
63.75
40.37
40.20
40.03
39.87
39.70
39.53
21.72
SO2Me
O
HO
N
N
Ts
O
6j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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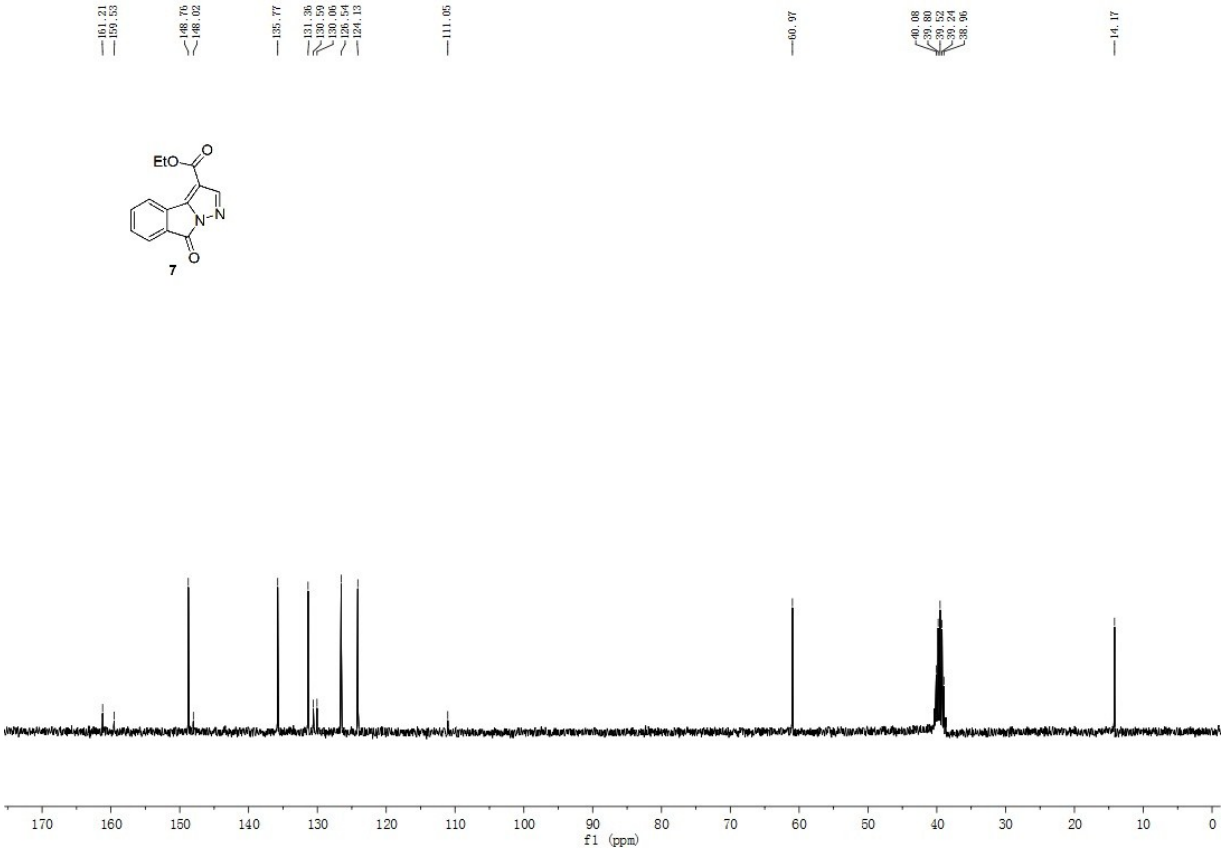
7.73
7.60
7.57
7.54
4.39
4.37
4.34
4.32
3.32
2.50
1.39
1.37
1.34
0.01
EtO
O
N
N
O
7
1.03
2.04
1.84
1.95
3.00
.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.36
130.59
130.06
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111.05
60.97
40.08
39.80
39.52
39.24
38.96
14.17
EtO
O
N
O
7
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)