

Supporting Online Material for

Copper catalyzed five-component domino strategy for the synthesis of nicotinimidamides

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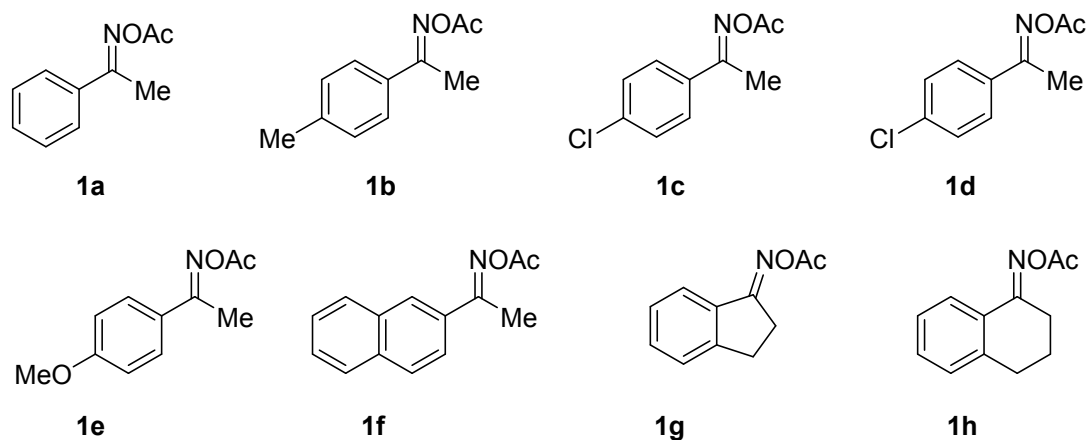
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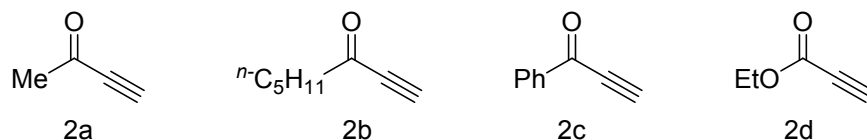
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1. The structures of starting materials **1a-1h**, **2a-2d**, **3a-3e** and **4a-4l**.

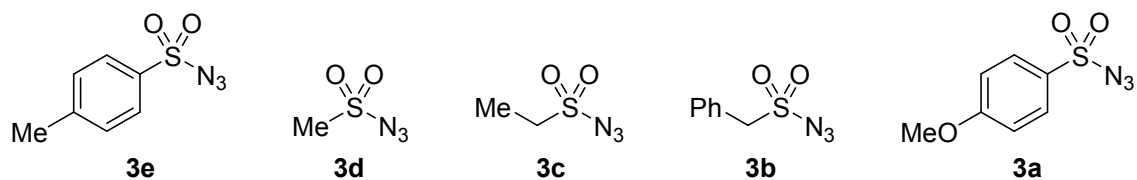
All oxime esters (**1a-1h**) prepared by literature methods¹.



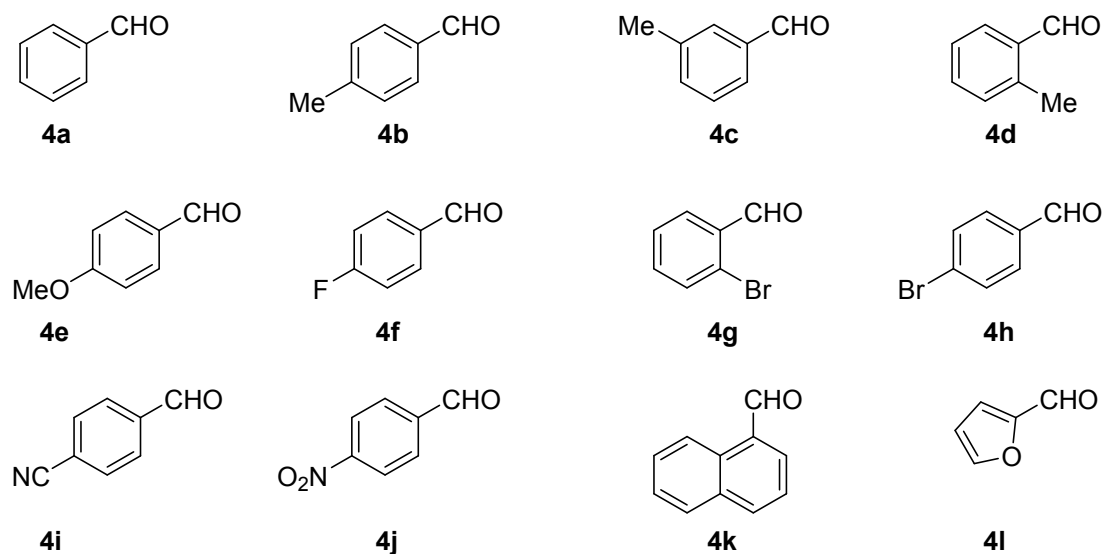
All terminal ynones (**2a-2d**) prepared by purchase or literature methods².



All oxime esters (**3a-3e**) prepared by literature methods³.



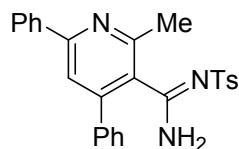
All aldehydes (**4a-4l**) prepared by purchase.



2. General Information

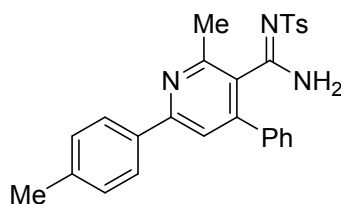
All melting points were determined on a Yanaco melting point apparatus and were uncorrected. IR spectra were recorded as KBr pellets on a Nicolet FT-IR 5DX spectrometer. All spectra of ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) were measured on a 400 MHz Bruker spectrometer using $\text{DMSO-}d_6$ or CDCl_3 as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. . Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. HRMS were obtained on a Bruker micrOTOF-Q II spectrometer.

3. Preparation and characterizations of compounds 6a-6z



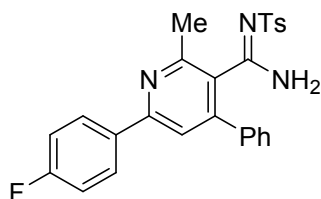
2-methyl-4,6-diphenyl-*N'*-tosylnicotinimidamide (6a). To a solution of (*E*)-1-phenylethan-1-one *O*-acetyl oxime (**1a**, 88.5 mg, 0.5 mmol), CuI (9.5 mg, 0.05 mmol), NH₄OAc (**5a**, 77.1 mg, 1.0 mmol) in MeCN (1 mL) was added. Then added the mixture But-3-yn-2-one (**2a**, 51.0 mg, 0.75 mmol), TsN₃ (**3a**, 147.8 mg, 0.75 mmol) and Benzaldehyde (**4a**, 79.5 mg, 0.75 mmol) in MeCN (2 mL). After the reaction stirred at 80 °C for 8 h, and cooled to room temperature, the solvent removed by evaporating in vacuum. The residue purified by a flash chromatography [silica gel, 20% EtOAc in petroleum ether (60–90 °C)] to give 172 mg (78%) of product **6a** as a white solid, mp 230-231 °C. IR (KBr) ν 3372, 3281, 1622, 1551, 1142, 1084 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.94 (s, 1H), 8.39 (s, 1H), 8.15 (d, *J* = 6.7 Hz, 2H), 7.74 (s, 1H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.52-7.44 (m, 5H), 7.39 (t, *J* = 7.4 Hz, 1H), 7.31-7.27 (m, 4H), 2.47 (s, 3H), 2.40 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.6, 155.6, 154.4, 147.7, 142.2, 137.9, 137.6, 129.4, 129.2 (3C), 128.7 (2C), 128.3 (2C), 128.2 (4C), 126.8 (2C), 126.2 (2C), 118.2, 22.2, 21.0; HRMS (ESI-TOF) (*m/z*). Calcd for C₂₆H₂₃N₃O₂S, [M+H]⁺ 442.1584; found 442.1580.

The products **6a-6z** prepared by the similar procedure.

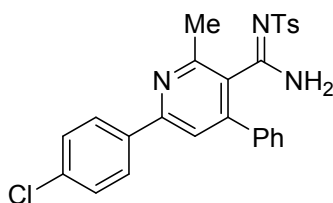


2-methyl-4-phenyl-6-(*p*-tolyl)-*N'*-tosylnicotinimidamide (6b). 182 mg (80%), white solid, mp 188-190 °C. IR (KBr) ν 3402, 3217, 1628, 1551, 1508, 1142, 1084 cm⁻¹; ¹H

NMR (400 MHz, DMSO-*d*₆) δ 8.98 (s, 1H), 8.44 (s, 1H), 8.06-8.04 (m, 2H), 7.68 (s, 1H), 7.54 (s, 2H), 7.43 (s, 2H), 7.30-7.29 (m, 5H), 7.06 (s, 2H), 2.48 (s, 3H), 2.40 (s, 3H), 2.36 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.7, 163.5, 161.0, 155.7, 154.3, 146.8, 142.4, 139.2, 135.2, 134.0, 130.3, 130.2, 129.4 (2C), 129.3 (2C), 128.2, 126.8 (2C), 126.3 (2C), 117.9, 115.2, 115.0, 22.3, 21.0, 20.9; HRMS (ESI-TOF) (*m/z*). Calcd for C₂₇H₂₅N₃O₂S, [M+H]⁺ 456.1740; found 456.1742.

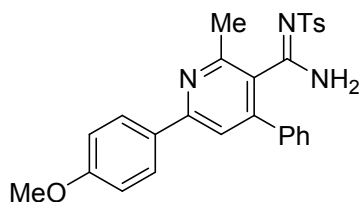


6-(4-fluorophenyl)-2-methyl-4-phenyl-*N'*-tosylnicotinimidamide (6c). 174 mg (76%), white solid, mp 225-227°C. IR (KBr) ν 3372, 3202, 1622, 1550, 1370, 1146 1084 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.94 (s, 1H), 8.40 (s, 1H), 8.22 (s, 2H), 7.75 (s, 1H), 7.54 (d, *J* = 6.9 Hz, 2H), 7.46 (d, *J* = 6.0 Hz, 2H), 7.38 (d, *J* = 6.9 Hz, 1H), 7.30 (d, *J* = 7.3 Hz, 6H), 2.46 (s, 3H), 2.40 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 164.4, 163.7, 162.0, 154.7, 154.5, 147.9, 142.4, 136.2 (d, *J* = 310.1 Hz), 129.3 (d, *J* = 2.4 Hz), 129.2 (3C), 129.1 (2C), 128.4, 128.3 (4C), 126.2 (3C), 118.2, 115.7 (d, *J* = 21.1 Hz), 22.3, 21.1; HRMS (ESI-TOF) (*m/z*). Calcd for C₂₆H₂₂FN₃O₂S, [M+H]⁺ 460.1490; found 460.1492.

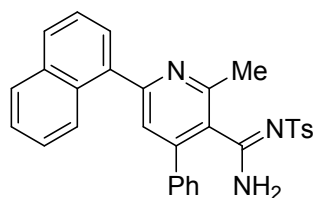


6-(4-chlorophenyl)-2-methyl-4-phenyl-*N'*-tosylnicotinimidamide (6d). 195 mg (82%), white solid, mp 234-235 °C. IR (KBr) ν 3441, 3264, 1628, 1551, 1281, 1150, 1092 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.93 (s, 1H), 8.40 (s, 1H), 8.20 (d, *J* = 8.4 Hz, 2H), 7.78 (s, 1H), 7.56-7.54 (m, 4H), 7.47 (d, *J* = 7.4 Hz, 2H), 7.40-7.34 (m, 1H), 7.31-7.26 (m, 4H), 2.47 (s, 3H), 2.40 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.6, 154.6, 154.4, 147.9, 142.4, 137.6, 136.8, 134.4, 129.4, 129.3 (2C), 128.9 (2C),

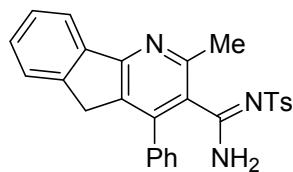
128.7 (3C), 128.5, 128.(3C), 126.3 (2C), 125.7, 118.4, 22.3, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $C_{26}H_{22}ClN_3O_2S$, $[M+H]^+$ 476.1194; found 476.1190.



6-(4-methoxyphenyl)-2-methyl-4-phenyl-*N'*-tosylnicotinimidamide (6e). 106 mg (45%), white solid, mp 226-228 °C. IR (KBr) ν 3364, 3312, 1586, 1550, 1254, 1146, 1084 cm^{-1} ; 1H NMR (400 MHz, $DMSO-d_6$) δ 8.92 (s, 1H), 8.36 (s, 1H), 8.11 (d, $J = 8.6$ Hz, 2H), 7.66 (s, 1H), 7.54 (d, $J = 7.8$ Hz, 2H), 7.45 (d, $J = 7.2$ Hz, 2H), 7.38 (t, $J = 7.2$ Hz, 1H), 7.30 (d, $J = 7.7$ Hz, 4H), 7.03 (d, $J = 8.6$ Hz, 2H), 3.81 (s, 3H), 2.44 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $DMSO-d_6$) δ 164.0, 160.6, 155.5, 154.3, 147.7, 142.4, 137.9, 130.5, 129.3 (3C), 128.4 (3C), 128.3 (4C), 127.7, 126.3 (2C), 117.4, 114.2 (2C), 55.4, 22.4, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $C_{27}H_{25}FN_3O_3S$, $[M+H]^+$ 472.1690; found 472.1691.

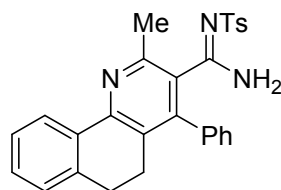


2-methyl-6-(naphthalen-1-yl)-4-phenyl-*N'*-tosylnicotinimidamide (6f). 182 mg (74%), white solid, mp 240-241 °C. IR (KBr) ν 3460, 3420, 1613, 1550, 1281, 1150 cm^{-1} ; 1H NMR (400 MHz, $DMSO-d_6$) δ 8.97 (s, 1H), 8.76 (s, 1H), 8.42 (s, 1H), 8.34 (d, $J = 8.6$ Hz, 1H), 8.07-8.02 (m, 2H), 7.97-7.94 (m, 2H), 7.56 (d, $J = 8.0$ Hz, 4H), 7.50 (d, $J = 7.2$ Hz, 2H), 7.41 (t, $J = 7.3$ Hz, 1H), 7.32 (t, $J = 7.5$ Hz, 4H), 2.52 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $DMSO-d_6$) δ 163.8, 155.5, 154.6, 147.9, 142.3, 137.7, 135.3, 133.5, 133.1, 129.3 (3C), 128.7, 128.5, 128.4, 128.3 (3C), 127.6 (2C), 127.0, 126.6, 126.4, 126.3 (3C), 124.5, 118.6, 22.4, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $C_{30}H_{25}N_3O_2S$, $[M+H]^+$ 492.1740; found 492.1744.



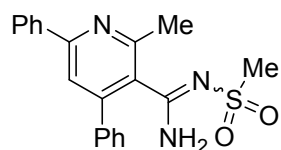
2-methyl-4-phenyl-*N'*-tosyl-5*H*-indeno[1,2-*b*]pyridine-3-carboximidamide (6g).

140 mg (62%), white solid, mp 103-105 °C. IR ν 3500, 3431, 1632, 1550, 1373, 1269, 1115 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.91 (s, 1H), 8.32 (s, 1H), 8.00 (d, $J = 7.0$ Hz, 1H), 7.59 (d, $J = 6.8$ Hz, 1H), 7.50-7.42 (m, 4H), 7.45-7.37 (m, 3H), 7.34-7.27 (m, 4H), 3.72 (s, 2H), 2.49 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 164.0, 159.2, 153.6, 144.6, 143.7, 142.2, 140.1, 135.7, 132.8, 129.4, 129.3 (2C), 129.1, 128.4, 128.3, 128.2 (2C), 127.9, 127.4, 126.2 (2C), 125.7 (2C), 120.7, 33.8, 22.2, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{23}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 454.1584; found 454.1581.



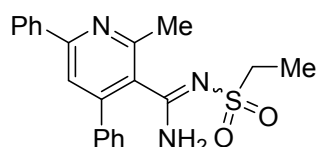
2-methyl-4-phenyl-*N'*-tosyl-5,6-dihydrobenzo[*h*]quinoline-3-carboximidamide

(6h). 124 mg (53%), white solid, mp 231-233 °C. IR (KBr) ν 3444, 3402, 1628, 1551, 1146, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.78 (s, 1H), 8.26 (d, $J = 7.0$ Hz, 2H), 7.48 (d, $J = 6.8$ Hz, 2H), 7.39-7.33 (m, 4H), 7.29-7.23 (m, 6H), 2.74 (t, $J = 6.1$ Hz, 2H), 2.50 (s, 2H), 2.43 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.6, 151.2, 151.1, 145.9, 142.1, 138.0, 135.5, 133.9, 129.5, 129.4, 129.2 (3C), 128.7, 128.0 (3C), 127.9 (2C), 127.0, 126.9, 126.1 (2C), 125.0, 27.1, 24.6, 22.1, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{28}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 468.1740; found 468.1736.

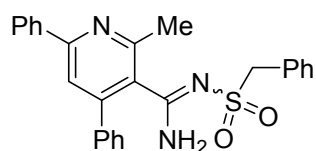


2-methyl-*N'*-(methylsulfonyl)-4,6-diphenylnicotinimidamide (6i). 104 mg (57%), white solid, mp 92 °C. IR (KBr) ν 3446, 3401, 2570, 1622, 1551, 1302, 1149, 1084

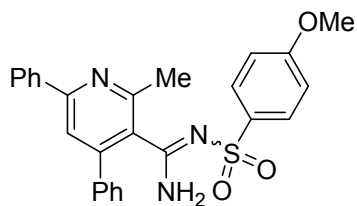
cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.88 (s, 1H), 8.24 (s, 1H), 8.15 (d, *J* = 7.7 Hz, 2H), 7.76 (s, 1H), 7.59 (d, *J* = 6.8 Hz, 2H), 7.52-7.44 (m, 6H), 2.62 (s, 6H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.9, 155.9, 154.6, 148.1, 138.2, 138.1, 129.6, 129.0 (2C), 128.7, 128.6 (4C), 127.1 (3C), 118.3, 22.6 (2C); HRMS (ESI-TOF) (*m/z*). Calcd for C₂₀H₁₉N₃O₂S, [M+H]⁺ 366.1271; found 366.1275



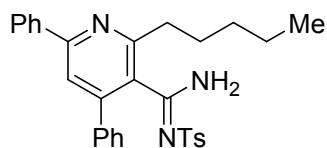
***N'*-(ethylsulfonyl)-2-methyl-4,6-diphenylnicotinimidamide (6j)**. 114 mg (60%), white solid, mp 98-100 °C. IR (KBr) ν 3449, 3372, 2570, 1622, 1551, 1447, 1269, 1111 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.87 (s, 1H), 8.25 (s, 1H), 8.16 (d, *J* = 7.0 Hz, 2H), 7.76 (s, 1H), 7.61 (d, *J* = 7.7 Hz, 2H), 7.53-7.44 (m, 6H), 2.74-2.64 (m, 2H), 2.69 (s, 3H), 0.96 (t, *J* = 7.2 Hz, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 164.0, 155.7, 154.5, 147.9, 138.1, 129.5, 128.9 (2C), 128.7, 128.6, 128.5 (2C), 128.4 (3C), 127.0 (2C), 118.3, 47.4, 22.6, 7.8; HRMS (ESI-TOF) (*m/z*). Calcd for C₂₁H₂₁N₃O₂S, [M+H]⁺ 380.1427; found 380.1424.



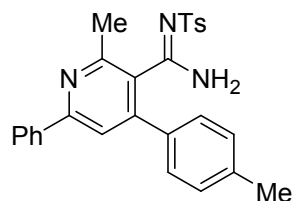
***N'*-(benzylsulfonyl)-2-methyl-4,6-diphenylnicotinimidamide (6k)**. 159 mg (72%), white solid, mp 148-150 °C. IR (KBr) ν 3445, 3310, 1601, 1551, 1451, 1285, 1254, 1119 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.83 (s, 1H), 8.27 (s, 1H), 8.16 (d, *J* = 7.0 Hz, 2H), 7.77 (s, 1H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.52-7.44 (m, 6H), 7.33-7.31 (m, 5H), 4.00 (s, 2H), 2.51 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 164.2, 155.7, 154.6, 147.9, 138.1, 138.0, 131.1 (2C), 130.2, 129.5, 128.9 (2C), 128.6 (3C), 128.5 (3C), 128.2 (2C), 127.9, 127.0 (2C), 118.2, 58.6, 22.5; HRMS (ESI-TOF) (*m/z*). Calcd for C₂₆H₂₃N₃O₂S, [M+H]⁺ 442.1584; found 442.1586.



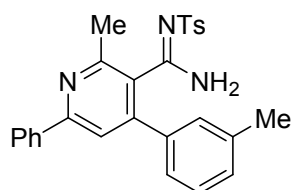
***N'*-((4-methoxyphenyl)sulfonyl)-2-methyl-4,6-diphenylnicotinimidamide (6l).** 91 mg (40%), white solid, mp 160-162 °C. IR (KBr) ν 3432, 3305.9, 1605.2, 1549.6, 1369.5, 1145.7, 1083.9 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.92 (s, 1H), 8.36 (s, 1H), 8.14 (d, $J = 7.0$ Hz, 2H), 7.73 (s, 1H), 7.61 (d, $J = 8.0$ Hz, 2H), 7.49 (d, $J = 7.3$ Hz, 5H), 7.38 (t, $J = 7.0$ Hz, 1H), 7.31 (d, $J = 7.0$ Hz, 2H), 7.00 (d, $J = 8.5$ Hz, 2H), 3.85 (3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.5, 162.1, 155.8, 154.6, 147.8, 138.1, 137.7, 129.5, 128.9 (2C), 128.5 (2C), 128.4 (2C), 128.3 (4C), 127.8, 127.0 (3C), 118.3, 114.1, 55.8, 22.4; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{26}\text{H}_{23}\text{N}_3\text{O}_3\text{S}$, $[\text{M}+\text{H}]^+$ 458.1533; found 458.1537.



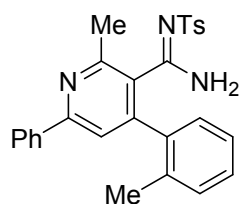
***(Z)*-2-pentyl-4,6-diphenyl-*N'*-tosylnicotinimidamide (6m).** 164 mg (66%), yellow oil. IR (KBr) ν 3406, 3221, 2928, 1624, 1498, 1146, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.93 (s, 1H), 8.35 (s, 1H), 8.15 (d, $J = 8.3$ Hz, 2H), 7.72 (s, 1H), 7.62 (d, $J = 7.8$ Hz, 2H), 7.51-7.45 (m, 5H), 7.39 (d, $J = 7.3$ Hz, 1H), 7.34-7.32 (m, 4H), 2.61 (t, $J = 8.0$ Hz, 2H), 2.40 (s, 3H), 1.68 (t, $J = 6.8$ Hz, 2H), 1.30-1.23 (m, 3H), 0.87 (t, $J = 7.0$ Hz, 4H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.6, 158.1, 155.7, 147.8, 142.4, 138.2, 137.8, 129.5, 129.3 (3C), 128.9 (2C), 128.5, 128.4 (2C), 128.3 (2C), 128.1, 126.9 (2C), 126.4 (2C), 118.2, 34.9, 31.4, 28.5, 22.1, 21.1, 14.0; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{30}\text{H}_{31}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 498.2210; found. 498.2213.



2-methyl-6-phenyl-4-(*p*-tolyl)-*N'*-tosylnicotinimidamide (6n). 189 mg (83%), white solid, mp 223-224 °C. IR (KBr) ν 3364, 3307, 1636, 1549, 1300, 1146, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.94 (s, 1H), 8.38 (s, 1H), 8.13 (d, $J = 6.7$ Hz, 2H), 7.70 (s, 1H), 7.56 (d, $J = 8.0$ Hz, 2H), 7.51-7.43 (m, 3H), 7.34 (t, $J = 8.4$ Hz, 4H), 7.05 (t, $J = 7.8$ Hz, 2H), 2.46 (s, 3H), 2.41 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.9, 155.7, 154.5, 147.8, 142.3, 138.1, 137.9, 134.8, 129.5, 129.3 (2C), 128.9 (3C), 128.8 (2C), 128.4, 128.1 (2C), 126.9 (2C), 126.4 (2C), 118.2, 22.3, 21.1, 21.0; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 456.1740; found 456.1744.

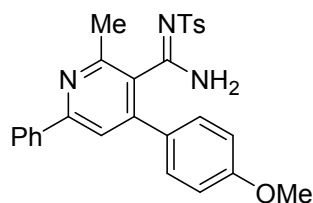


2-methyl-6-phenyl-4-(*m*-tolyl)-*N'*-tosylnicotinimidamide (6o). 184 mg (81%), white solid, mp 221-222 °C. IR (KBr) ν 3451, 1628, 1549, 1308, 1146, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.94 (s, 1H), 8.39 (s, 1H), 8.15 (d, $J = 6.7$ Hz, 2H), 7.73 (s, 1H), 7.56-7.45 (m, 5H), 7.37-7.25 (m, 4H), 7.21-7.14 (m, 2H), 2.48 (s, 3H), 2.39 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.8, 155.7, 154.4, 147.9, 142.3, 138.1, 137.7, 137.6, 129.5, 129.4, 129.3 (2C), 129.1, 128.8 (2C), 128.5, 128.2, 127.0 (2C), 126.2 (2C), 125.7, 125.3, 118.3, 22.4, 21.1, 21.0; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 456.1740; found 456.1742.

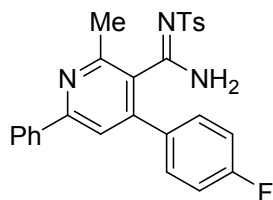


2-methyl-6-phenyl-4-(*o*-tolyl)-*N'*-tosylnicotinimidamide (6p). 178 mg (78%), white

solid, mp 192-195 °C. IR (KBr) ν 3395, 3310, 3229, 1636, 1550, 1279, 1142, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.86 (s, 1H), 8.22 (s, 1H), 8.11 (d, $J = 6.7$ Hz, 2H), 7.61 (s, 1H), 7.48-7.43 (m, 5H), 7.27-7.21 (m, 3H), 7.14 (t, $J = 7.4$ Hz, 2H), 7.04 (t, $J = 7.0$ Hz, 1H), 2.48 (s, 3H), 2.39 (s, 3H), 2.03 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.2, 155.1, 154.4, 147.9, 142.2, 139.1, 138.0, 136.9, 135.3, 130.0, 129.5, 129.3, 129.2 (2C), 128.9 (2C), 128.6, 128.1, 126.9 (2C), 126.0 (2C), 125.0, 118.5, 22.3, 21.1, 20.0; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 456.1740; found 456.1745.

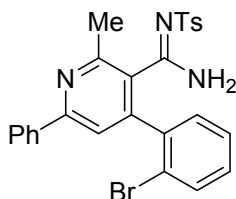


4-(4-methoxyphenyl)-2-methyl-6-phenyl-*N'*-tosylnicotinimidamide (6q). 155 mg (66%), white solid, mp 220-221 °C. IR (KBr) ν 3364, 3310, 1635, 1549, 1300, 1146, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.96 (s, 1H), 8.41 (s, 1H), 8.13 (d, $J = 6.8$ Hz, 2H), 7.70 (s, 1H), 7.58 (d, $J = 7.8$ Hz, 2H), 7.51-7.45 (m, 3H), 7.39 (d, $J = 8.4$ Hz, 2H), 7.31 (d, $J = 8.1$ Hz, 2H), 6.79 (d, $J = 8.4$ Hz, 2H), 3.79 (s, 3H), 2.47 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 164.1, 160.0, 155.7, 154.5, 147.4, 142.4, 139.1, 138.2, 129.9 (2C), 129.6 (2C), 129.4, 129.3 (2C), 128.8 (2C), 128.4, 126.9 (2C), 126.4 (2C), 118.2, 113.7, 55.2, 22.3, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{25}\text{N}_3\text{O}_3\text{S}$, $[\text{M}+\text{H}]^+$ 472.1690; found 472.1693.

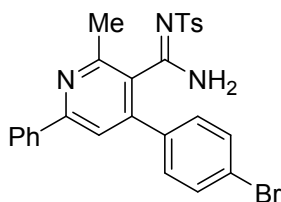


4-(4-fluorophenyl)-2-methyl-6-phenyl-*N'*-tosylnicotinimidamide (6r). 174 mg (76%), white solid, mp 169-171 °C. IR (KBr) ν 3372, 3283, 1622, 1550, 1370, 1146, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 9.01 (s, 1H), 8.45 (s, 1H), 8.14 (d, $J = 6.6$ Hz, 2H), 7.73 (s, 1H), 7.55 (d, $J = 8.9$ Hz, 2H), 7.51-7.42 (m, 5H), 7.30 (d, $J = 8.0$

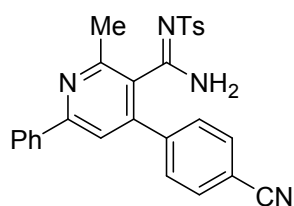
Hz, 2H), 7.06 (t, $J = 8.5$ Hz, 2H), 2.49 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 163.6, 162.3 (d, $J = 243.9$ Hz), 155.8, 154.5, 146.9, 142.4, 138.0, 134.0 (d, $J = 1.0$ Hz), 130.3 (d, $J = 8.1$ Hz), 129.5, 129.3 (3C), 128.9 (3C), 128.5, 127.0 (3C), 126.3 (2C), 118.3, 115.1 (d, $J = 21.4$ Hz), 22.3, 21.0; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{26}\text{H}_{22}\text{FN}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 460.1490; found 460.1492.



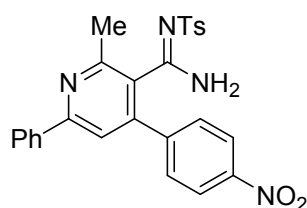
4-(2-bromophenyl)-2-methyl-6-phenyl- N' -tosylnicotinimidamide (6s). 156 mg (60%), white solid, mp 126-128 °C. IR (KBr) ν 3400, 3264, 1632, 1555, 1310, 1153, 1092 cm^{-1} ; ^1H NMR (400 MHz, DMSO- d_6) δ 8.95 (s, 1H), 8.30 (s, 1H), 8.10 (d, $J = 9.6$ Hz, 2H), 7.66 (s, 1H), 7.55 (d, $J = 8.0$ Hz, 1H), 7.50-7.43 (m, 5H), 7.29-7.19 (m, 5H), 2.53 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 162.6, 155.1, 154.6, 147.0, 142.2, 138.8, 137.8, 137.6, 132.6, 130.4, 130.1, 129.6, 129.2 (2C), 128.9 (3C), 126.9, 126.8 (2C), 126.0 (2C), 121.9, 118.9, 22.3, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{26}\text{H}_{22}\text{BrN}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 520.0689; found 520.0692.



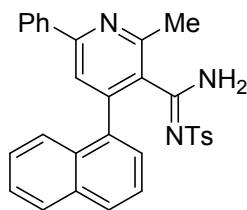
4-(4-bromophenyl)-2-methyl-6-phenyl- N' -tosylnicotinimidamide (6t). 195 mg (75%), white solid, mp 241-243 °C. IR (KBr) ν 3364, 3063, 1628, 1549, 1308, 1150, 1084 cm^{-1} ; ^1H NMR (400 MHz, DMSO- d_6) δ 8.96 (s, 1H), 8.30 (s, 1H), 8.10 (d, $J = 6.6$ Hz, 2H), 7.66 (s, 1H), 7.55 (d, $J = 8.5$ Hz, 1H), 7.50-7.43 (m, 5H), 7.29-7.19 (m, 5H), 2.53 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 163.0, 155.5, 155.0, 147.4, 142.6, 139.2, 138.2, 138.0, 133.0, 130.8, 130.5, 130.0, 129.6 (2C), 129.3 (3C), 127.3, 127.2 (2C), 126.4 (2C), 122.3, 119.3, 22.7, 21.5; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{26}\text{H}_{22}\text{BrN}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 520.0689; found 520.0693.



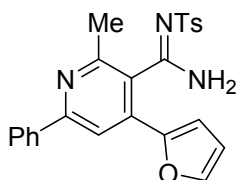
4-(4-cyanophenyl)-2-methyl-6-phenyl-*N'*-tosylnicotinimidamide (6u). 172 mg (74%), white solid, mp 226-227 °C. IR (KBr) ν 3395, 3298, 2230, 1628, 1443, 1080 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 9.12 (s, 1H), 8.52 (s, 1H), 8.14 (d, $J = 7.0$ Hz, 2H), 7.76 (s, 1H), 7.62 (s, 2H), 7.53-7.46 (m, 7H), 7.29 (d, $J = 7.7$ Hz, 2H), 2.55 (s, 3H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.2, 156.1, 154.8, 146.5, 142.7, 142.3, 137.9, 132.1 (2C), 129.8, 129.4 (3C), 129.1, 129.0 (3C), 128.3, 127.1 (2C), 126.5 (2C), 118.8, 118.1, 111.2, 22.5, 21.2; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{22}\text{N}_4\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 467.1536; found 467.1533.



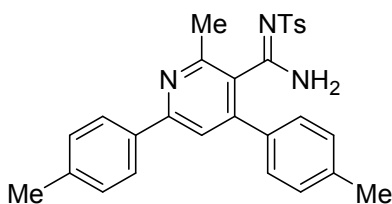
2-methyl-4-(4-nitrophenyl)-6-phenyl-*N'*-tosylnicotinimidamide (6v). 102 mg (42%), white solid, mp 233-234 °C. IR (KBr) ν 3429, 3400, 1628, 1551, 1350, 1142, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 9.14 (s, 1H), 8.54 (s, 1H), 8.16 (d, $J = 6.9$ Hz, 2H), 7.98 (d, $J = 6.2$ Hz, 2H), 7.80 (s, 1H), 7.58 (d, $J = 6.6$ Hz, 2H), 7.53-7.46 (m, 5H), 7.23 (d, $J = 7.6$ Hz, 2H), 2.58 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.0, 156.0, 154.7, 147.1, 146.0, 144.2, 142.5, 137.7, 129.7, 129.5 (2C), 129.2 (3C), 128.9 (2C), 128.2, 127.0 (2C), 126.4 (2C), 123.2 (2C), 118.0, 22.4, 20.9; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{26}\text{H}_{22}\text{N}_4\text{O}_4\text{S}$, $[\text{M}+\text{H}]^+$ 487.1435; found 487.1433.



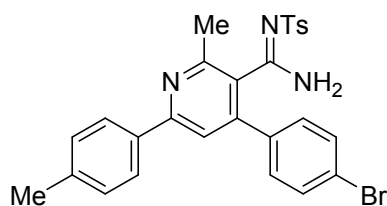
2-methyl-4-(naphthalen-1-yl)-6-phenyl-*N'*-tosylnicotinimidamide (6w). 164 mg (67%), white solid, mp 215-217 °C. IR (KBr) ν 3368, 3313, 1624, 1543, 1304, 1157, 1084 cm^{-1} ; ^1H NMR (400 MHz, DMSO- d_6) δ 9.03 (s, 1H), 8.41 (s, 1H), 8.17 (d, J = 6.8 Hz, 2H), 8.04 (s, 1H), 7.94 (d, J = 7.4 Hz, 1H), 7.86 (s, 1H), 7.79 (d, J = 7.7 Hz, 2H), 7.62-7.55 (m, 3H), 7.53-7.46 (m, 3H), 7.43 (d, J = 8.2 Hz, 2H), 7.05 (d, J = 8.0 Hz, 2H), 2.53 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 163.8, 155.8, 154.6, 147.8, 142.2, 138.1, 135.3, 132.7, 132.6, 129.6, 129.1 (3C), 128.9 (2C), 128.7, 128.3, 127.8, 127.7, 127.6, 127.0 (2C), 126.8, 126.6, 126.1 (2C), 126.0, 118.6, 22.4, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{30}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 492.1740; found 492.1742.



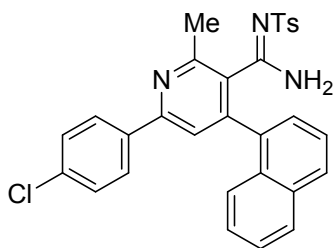
4-(furan-2-yl)-2-methyl-6-phenyl-*N'*-tosylnicotinimidamide (6x). 129 mg (60%), white solid, mp 135-137 °C. IR (KBr) ν 3372, 3275, 3210, 1624, 1546, 1308, 1150, 1084 cm^{-1} ; ^1H NMR (400 MHz, DMSO- d_6) δ 8.99 (s, 1H), 8.62 (s, 1H), 8.14 (d, J = 7.2 Hz, 2H), 8.04 (s, 1H), 7.71-7.64 (m, 3H), 7.54-7.46 (m, 3H), 7.32 (d, J = 7.0 Hz, 2H), 7.03 (s, 1H), 6.59-6.58 (m, 1H), 2.40 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, DMSO- d_6) δ 155.9, 155.1, 148.9, 144.8, 142.4, 138.0, 135.2, 129.6, 129.3 (2C), 128.9 (3C), 126.8 (3C), 126.5 (2C), 112.8, 112.5, 112.0, 22.2, 21.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{24}\text{H}_{21}\text{N}_3\text{O}_3\text{S}$, $[\text{M}+\text{H}]^+$ 432.1377; found 432.1375.



2-methyl-4,6-di-*p*-tolyl-*N'*-tosylnicotinimidamide (6y). 190 mg (81%), white solid, mp 144–146 °C. IR (KBr) ν 3391, 3267, 1447, 1304, 1153, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.92 (s, 1H), 8.37 (s, 1H), 8.04 (d, $J = 8.1$ Hz, 2H), 7.66 (s, 1H), 7.56 (d, $J = 7.8$ Hz, 2H), 7.34–7.28 (m, 6H), 7.05 (d, $J = 7.7$ Hz, 2H), 2.45 (s, 3H), 2.41 (s, 3H), 2.36 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 164.0, 155.7, 154.3, 147.6, 142.3, 139.1, 137.8, 135.3, 134.9, 129.4 (2C), 129.2 (3C), 128.9 (3C), 128.1 (2C), 126.8 (2C), 126.4 (2C), 117.8, 22.3, 21.1, 20.9, 20.8; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{30}\text{H}_{25}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 470.1897; found 470.1893.

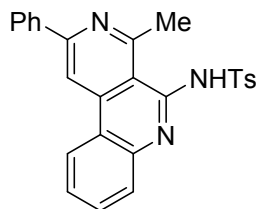


4-(4-bromophenyl)-2-methyl-6-(*p*-tolyl)-*N'*-tosylnicotinimidamide (6z). 195 mg (73%), white solid, mp 162.3–165.2 °C. IR (KBr) ν 3402, 3200, 1628, 1490, 1277, 1142, 1084 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.98 (s, 1H), 8.42 (s, 1H), 8.05 (d, $J = 8.2$ Hz, 2H), 7.69 (s, 1H), 7.55 (d, $J = 8.0$ Hz, 2H), 7.39 (d, $J = 7.7$ Hz, 2H), 7.31 (t, $J = 7.3$ Hz, 6H), 2.50 (s, 3H), 2.43 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.5, 155.9, 154.5, 146.7, 142.5, 139.3, 136.9, 135.2, 131.1 (3C), 130.2, 129.5 (2C), 129.3 (3C), 128.0, 126.9 (2C), 126.4 (2C), 122.1, 117.7, 22.4, 21.2, 21.0; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{27}\text{H}_{24}\text{BrN}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 534.0846; found 534.0848.



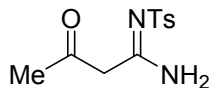
6-(4-chlorophenyl)-2-methyl-4-(naphthalen-1-yl)-N'-tosylnicotinimidamide (6aa).

184 mg (70%), white solid, mp 126-128 °C. IR (KBr) ν 3400, 3200, 1632, 1450, 1273, 1089 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 9.03 (s, 1H), 8.42 (s, 1H), 8.23 (d, $J = 7.5$ Hz, 2H), 8.04 (s, 1H), 7.94 (d, $J = 7.6$ Hz, 1H), 7.91 (s, 1H), 7.79 (d, $J = 7.5$ Hz, 2H), 7.62-7.55 (m, 5H), 7.43 (d, $J = 7.2$ Hz, 2H), 7.04 (d, $J = 7.6$ Hz, 2H), 2.52 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) δ 163.7, 154.7, 154.5, 148.0, 142.2, 136.8, 135.2, 134.4, 132.7, 132.6, 129.1 (3C), 129.0 (2C), 128.9, 128.8 (2C), 128.3, 127.8 (2C), 127.6, 126.8, 126.6, 126.1 (2C), 126.0, 118.6, 22.4, 22.1; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{30}\text{H}_{24}\text{ClN}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 526.1351; found 526.1355.



4-methyl-N-(4-methyl-2-phenylbenzo[c][2,7]naphthyridin-5-

yl)benzenesulfonamide (6ab). 200 mg (91%), white solid, mp 241-243 °C. IR (KBr) ν 3433, 3170, 1624, 1574, 1497, 1411, 1388 cm^{-1} ; ^1H NR (400 MHz, CDCl_3) δ 11.87 (s, 1H), 8.36 (s, 1H), 8.32 (d, $J = 8.1$ Hz, 1H), 8.17 (d, $J = 8.2$ Hz, 2H), 7.95 (d, $J = 8.3$ Hz, 2H), 7.63 (t, $J = 7.3$ Hz, 1H), 7.55-7.49 (m, 3H), 7.42 (t, $J = 7.7$ Hz, 1H), 7.33 (t, $J = 8.7$ Hz, 3H), 3.16 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 163.5, 158.0, 153.1, 143.1, 142.5, 140.1, 138.4, 134.9, 132.2, 130.2, 129.6 (2C), 129.1 (2C), 127.8 (2C), 126.3 (2C), 124.8, 123.8, 118.1, 117.4, 117.0, 110.0, 30.0, 21.7; HRMS (ESI-TOF) (m/z). Calcd for $\text{C}_{26}\text{H}_{21}\text{N}_3\text{O}_2\text{S}$, $[\text{M}+\text{H}]^+$ 440.1427; found 440.1430.



3-oxo-*N'*-tosylbutanimidamide (7a). To a solution of NH₄OAc (0.77g, 10 mmol), CuI (0.19 g, 1.0 mmol), TsN₃ (**3a**, 2.37 g, 12 mmol) in MeCN (15 mL) was added. Then added the but-3-yn-2-one (**2a**, 0.82 g, 12 mmol) slowly within 30 min at 0 °C. After the reaction was stirred at 0 °C for 1 h, room temperature for 12 h, the mixture was evaporated in vacuum. The residue was purified by a flash chromatography [silica gel, 50% EtOAc in petroleum ether (60–90 °C)] to give 1.57 g (62%) of product **5** as a white solid, mp 128–129 °C. IR (KBr) ν 3433, 3352, 3060, 2923, 1518, 1144 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.52 (s, 1H), 8.18 (s, 1H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 2H), 3.54 (s, 2H), 2.35 (s, 3H), 2.10 (s, 3H); ¹³C NMR (400 MHz, DMSO-*d*₆) δ 201.4, 163.7, 142.1, 140.0, 129.2 (2C), 126.0 (2C), 49.8, 29.8, 21.0; HRMS (ESI-TOF) (*m/z*). Calcd for C₁₁H₁₄N₂O₃S, [M+H]⁺ 255.0798; found 255.0795.

4. NMR Spectra

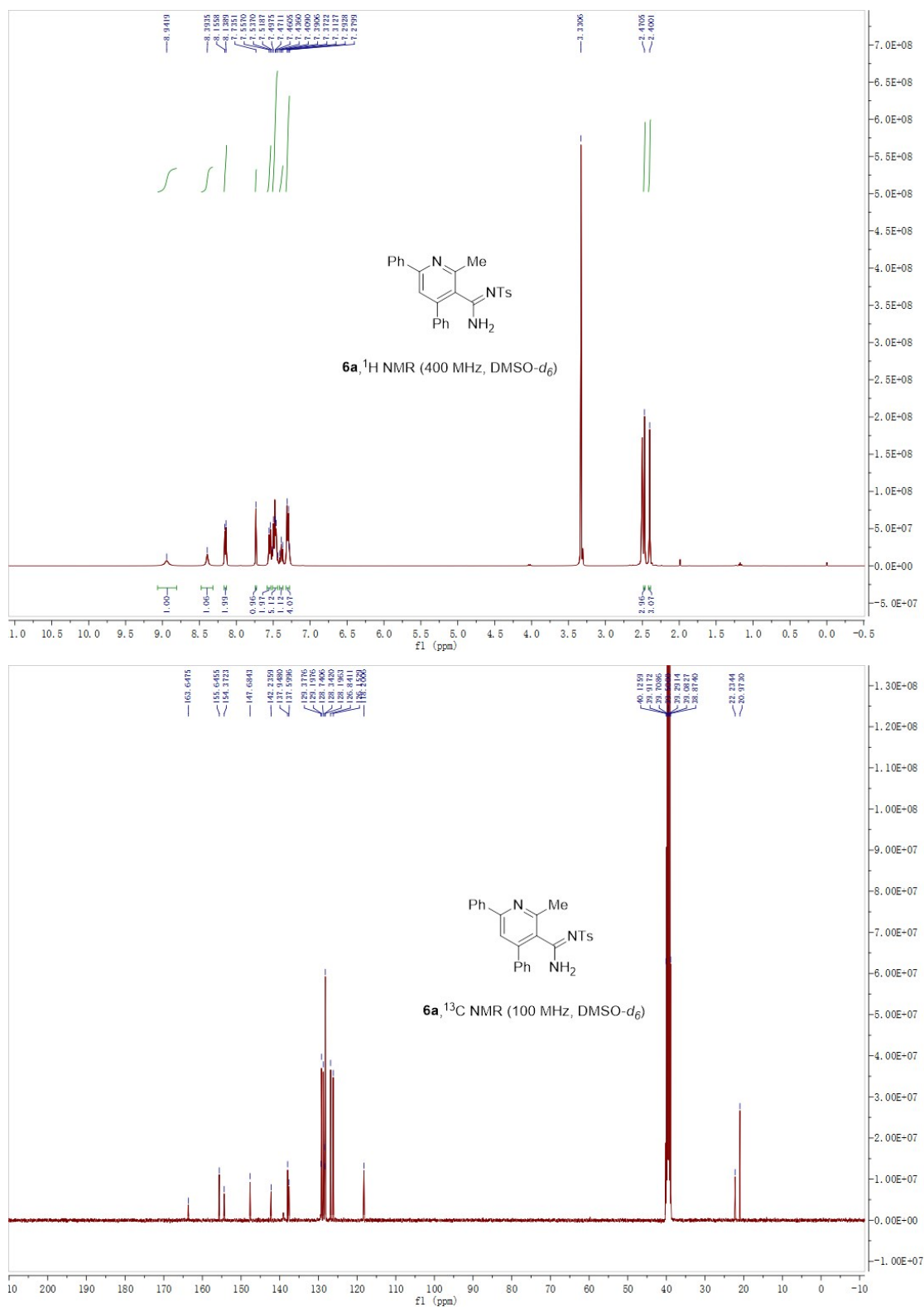


Figure S1. ^1H NMR of **6a** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6a** (100 MHz, $\text{DMSO-}d_6$).

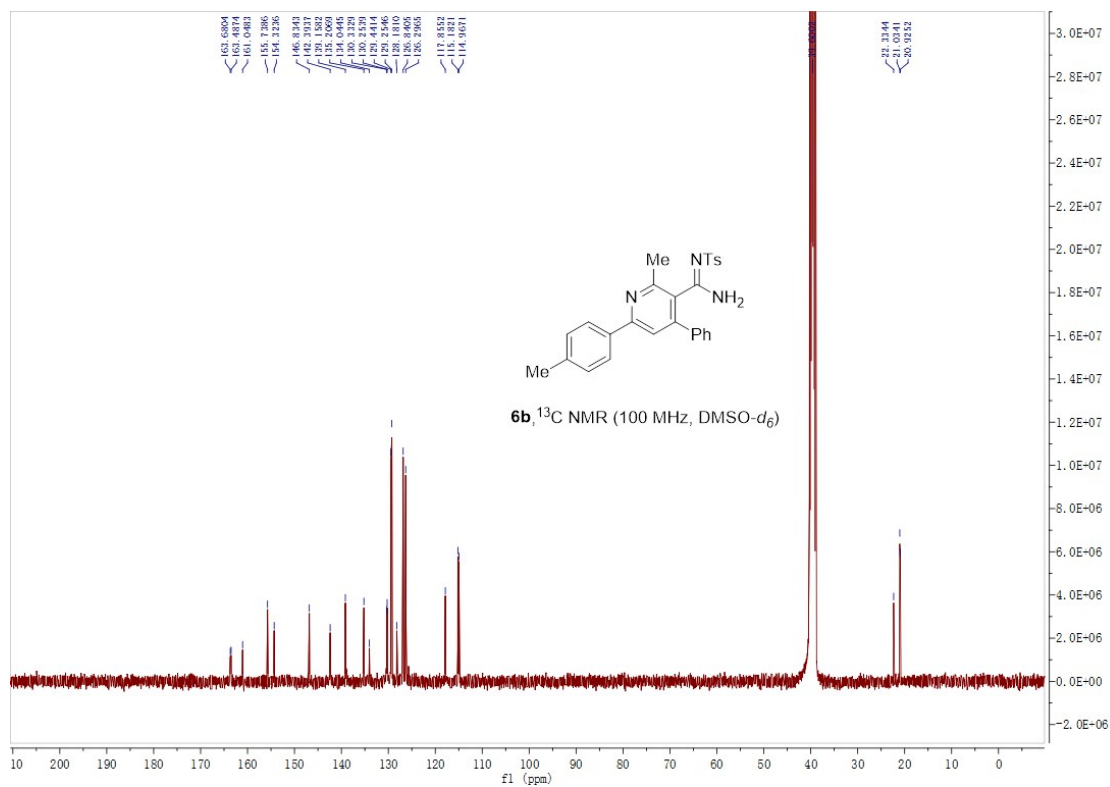
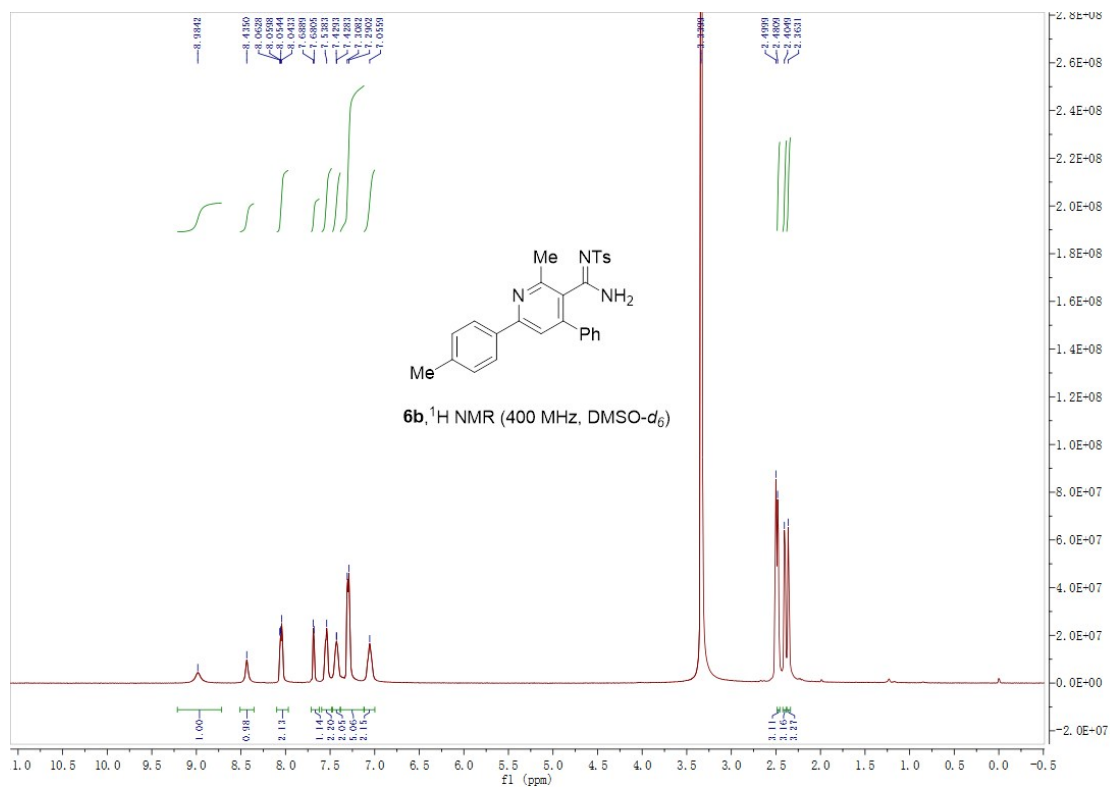


Figure S2. ¹H NMR of **6b** (400 MHz, DMSO-*d*₆) and ¹³C NMR of **6b** (100 MHz, DMSO-*d*₆).

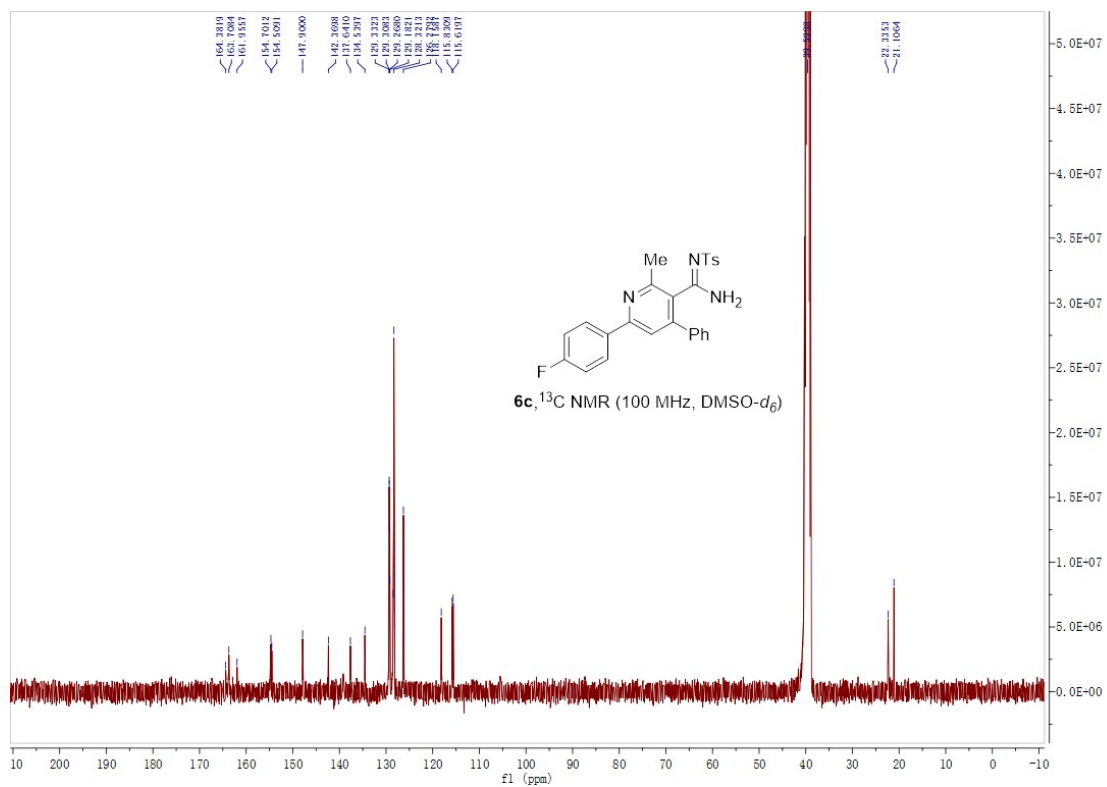
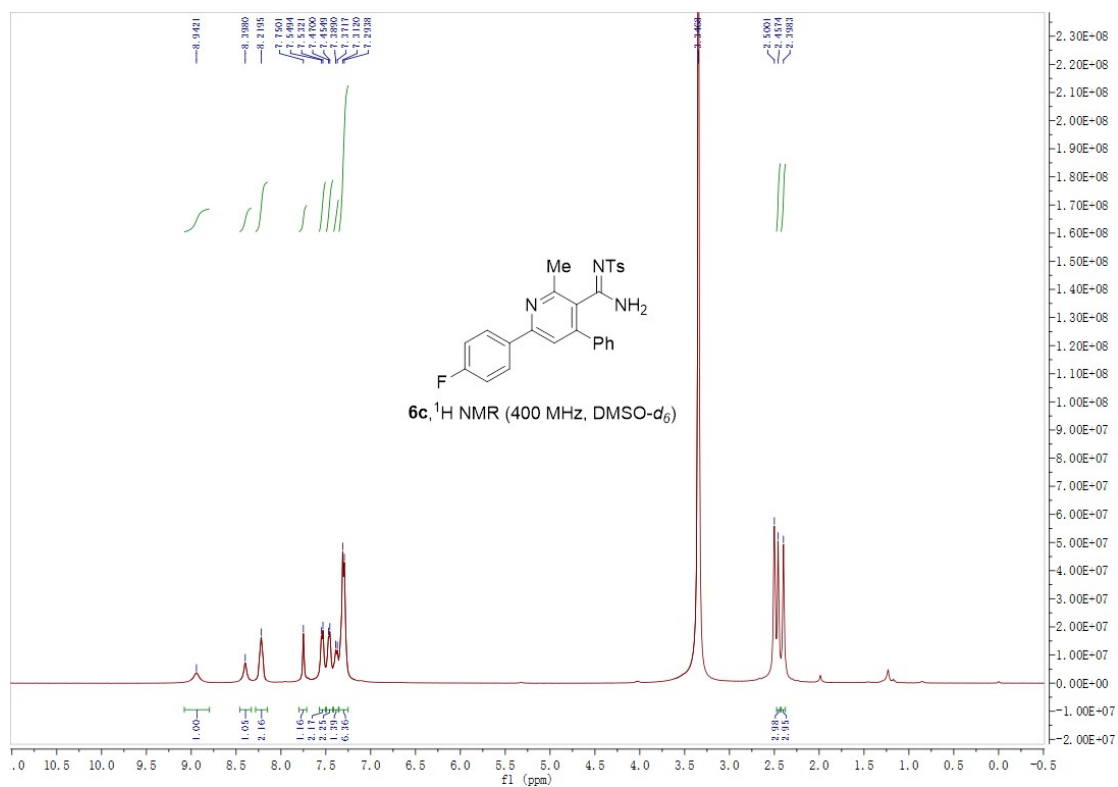


Figure S3. ^1H NMR of **6c** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6c** (100 MHz, $\text{DMSO-}d_6$).

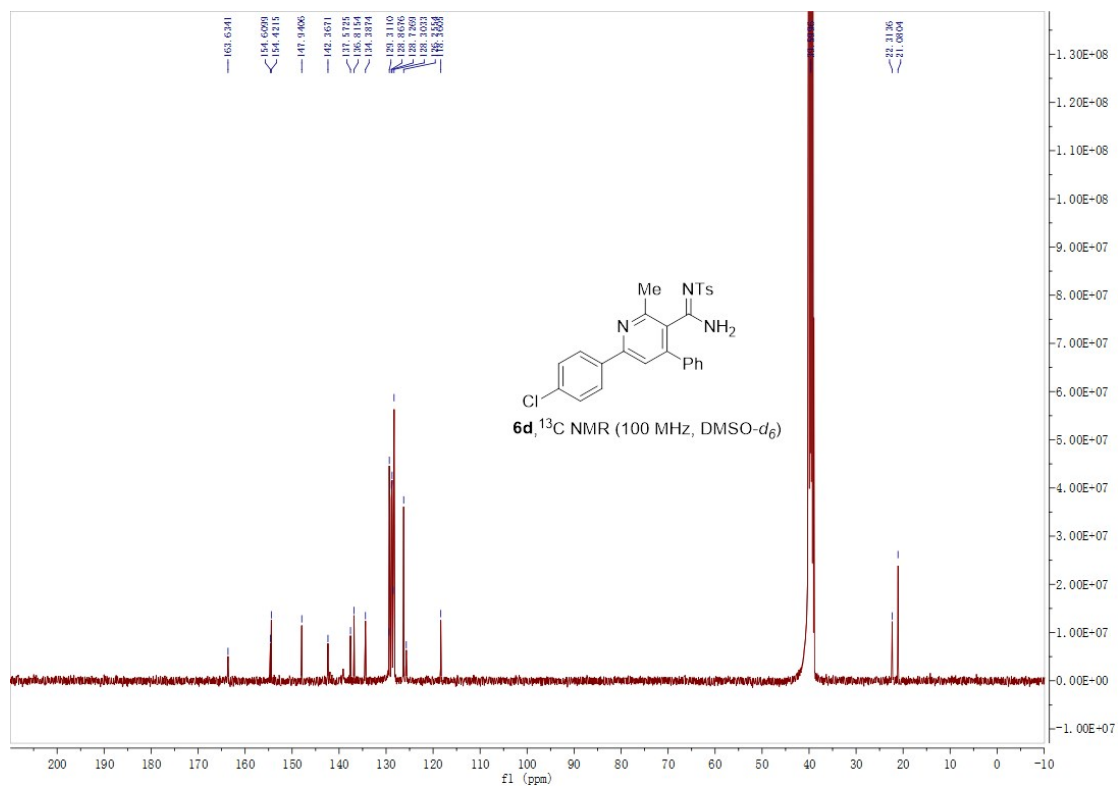
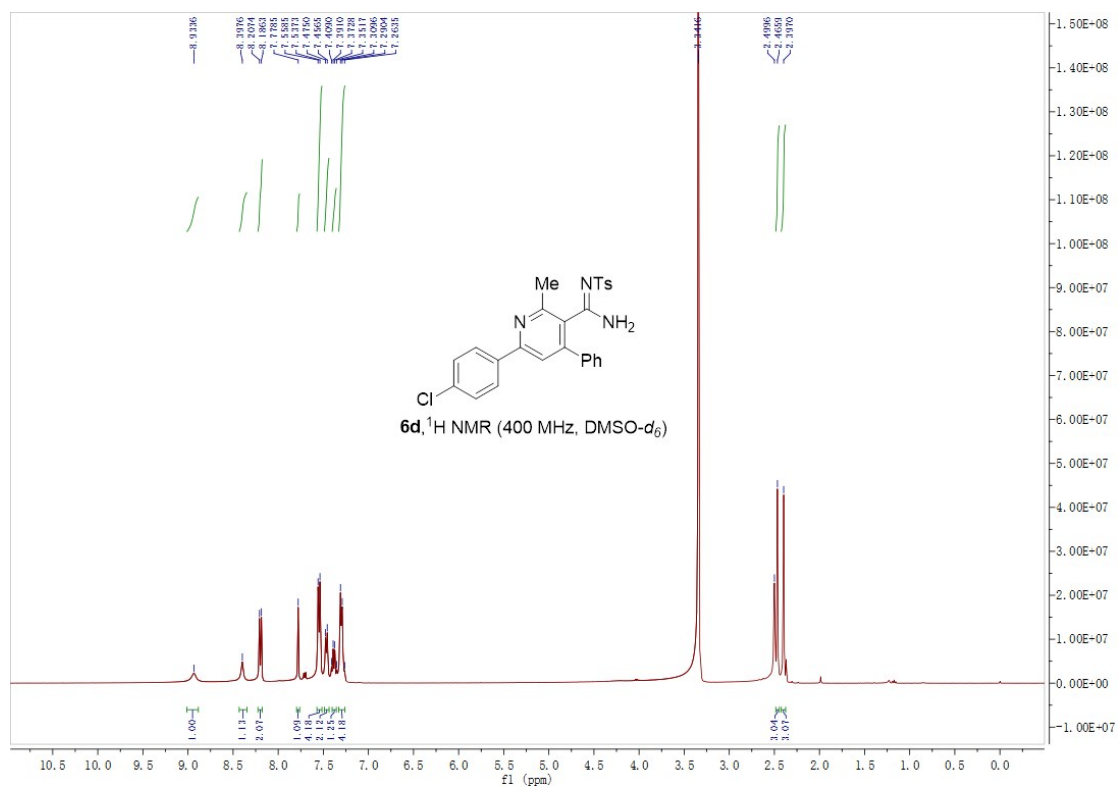


Figure S4. ^1H NMR of **6d** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6d** (100 MHz, $\text{DMSO-}d_6$).

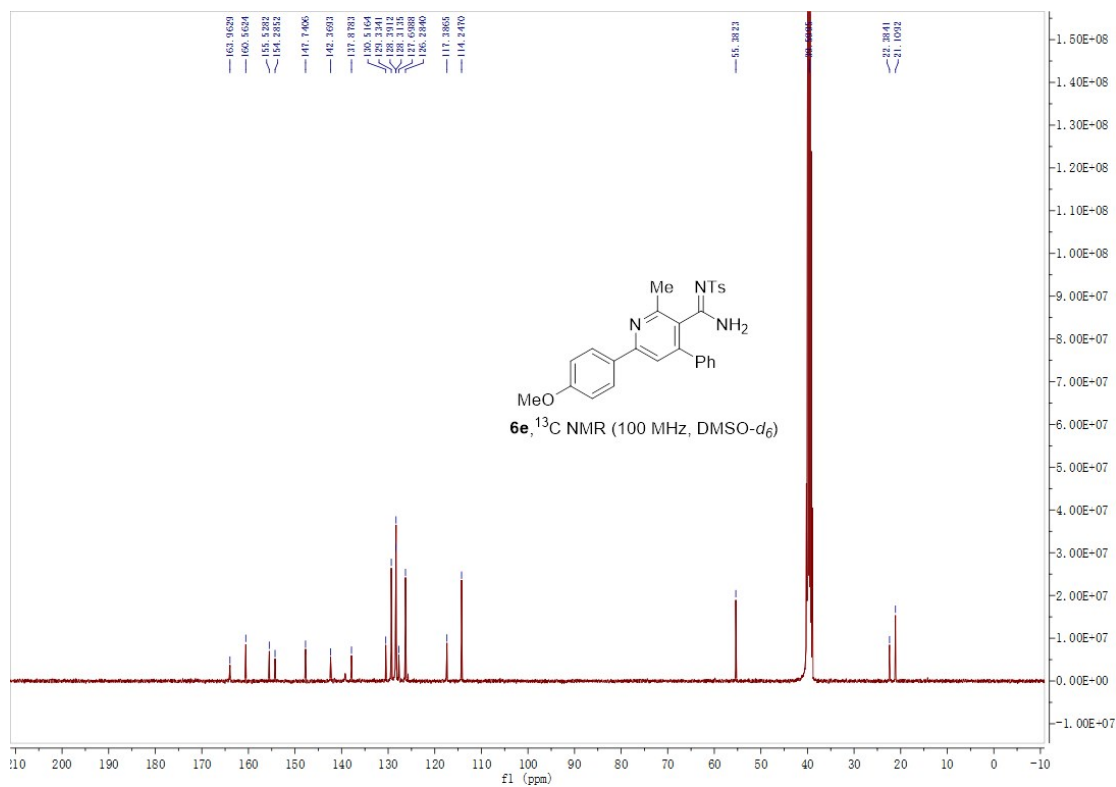
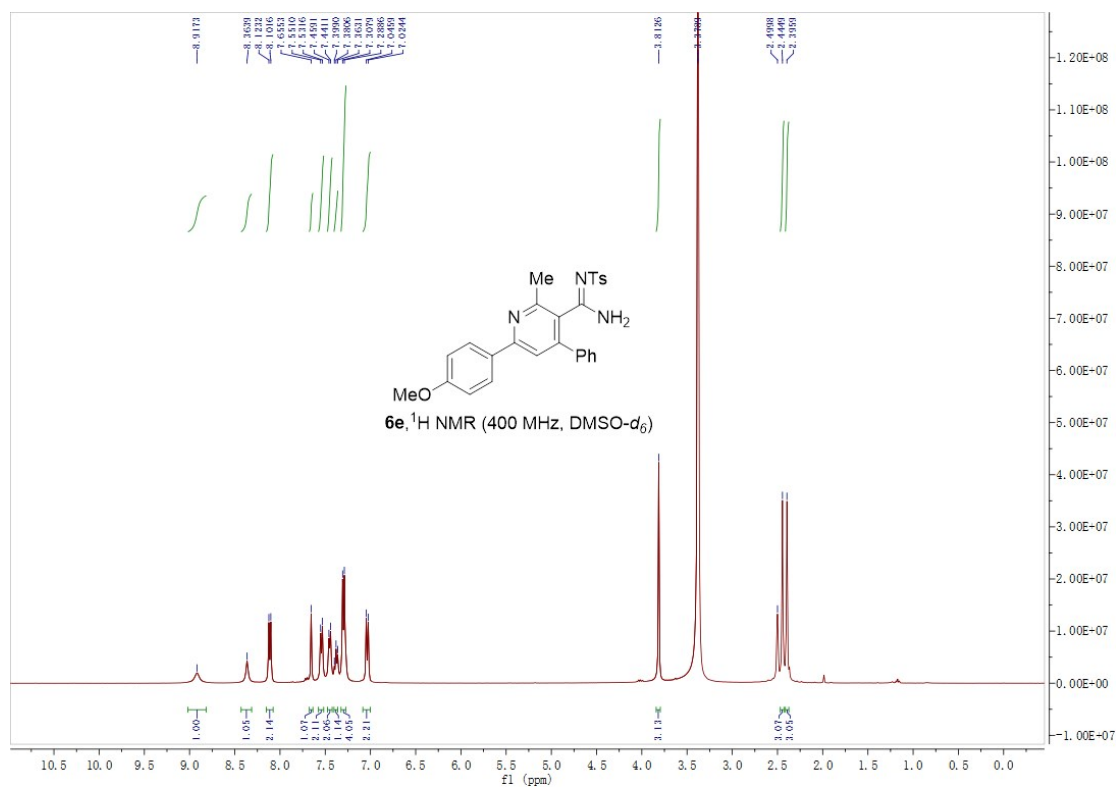


Figure S5. ^1H NMR of **6e** (400 MHz, $\text{DMSO}-d_6$) and ^{13}C NMR of **6e** (100 MHz, $\text{DMSO}-d_6$).

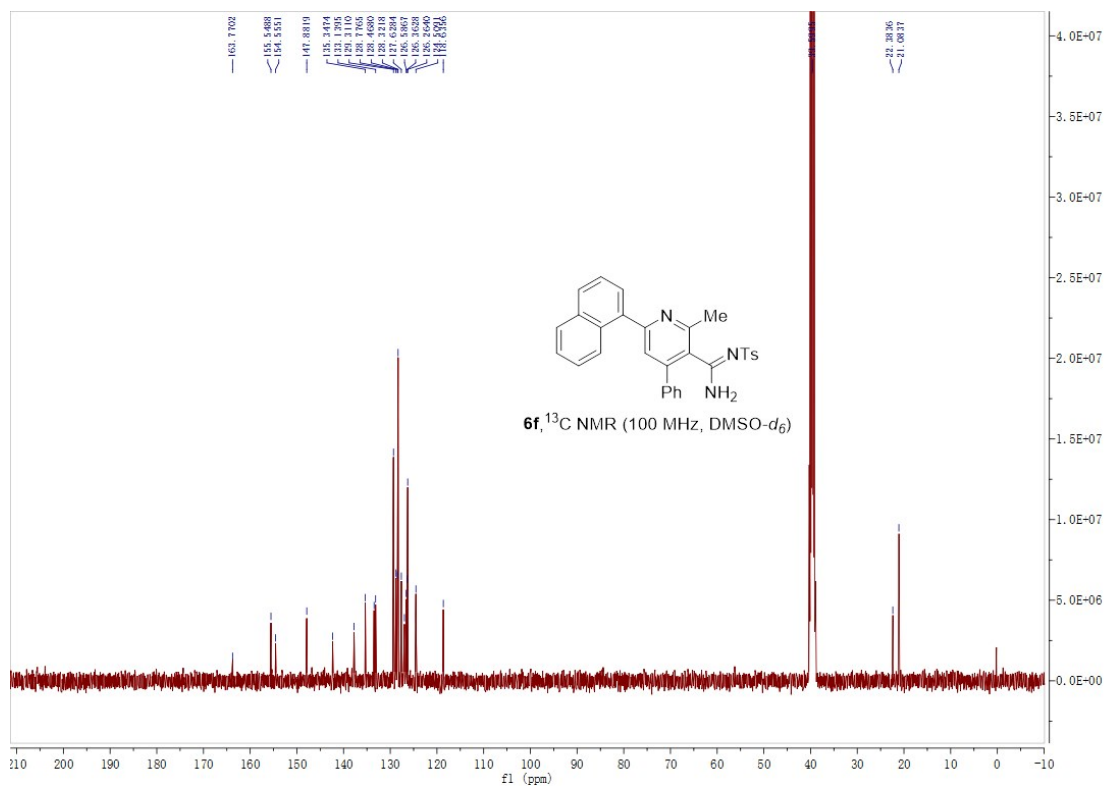
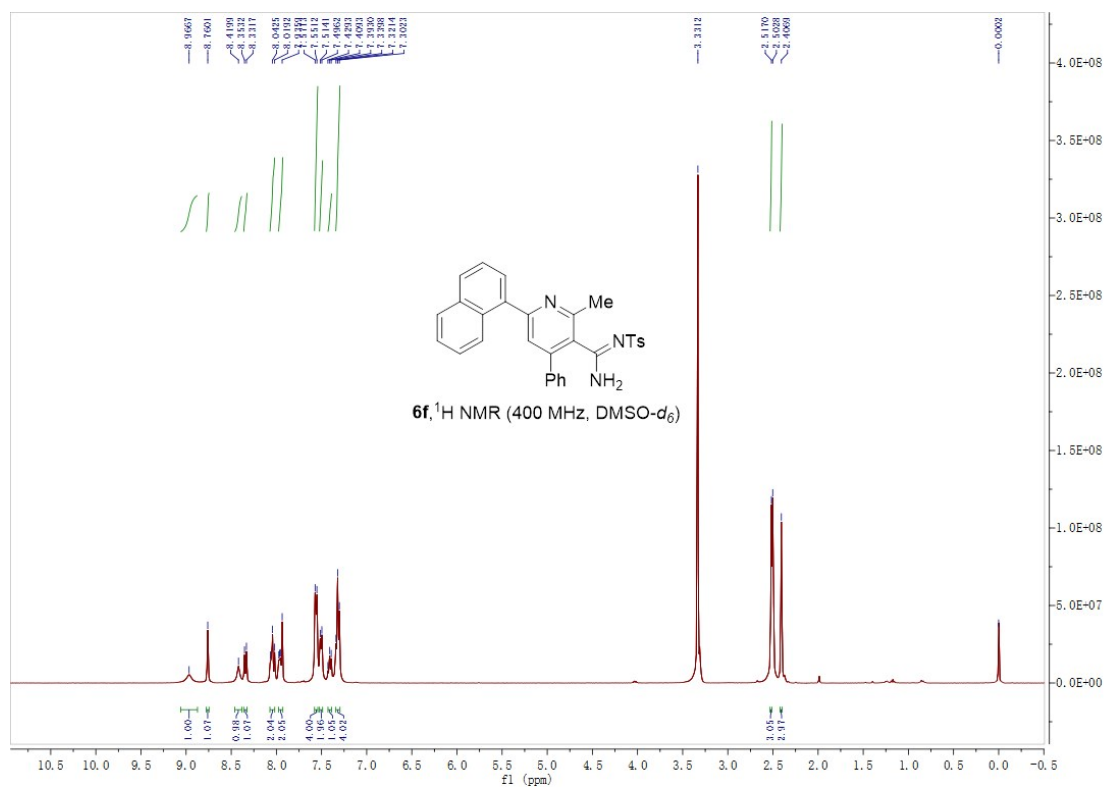


Figure S6. ^1H NMR of **6f** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6f** (100 MHz, $\text{DMSO-}d_6$).

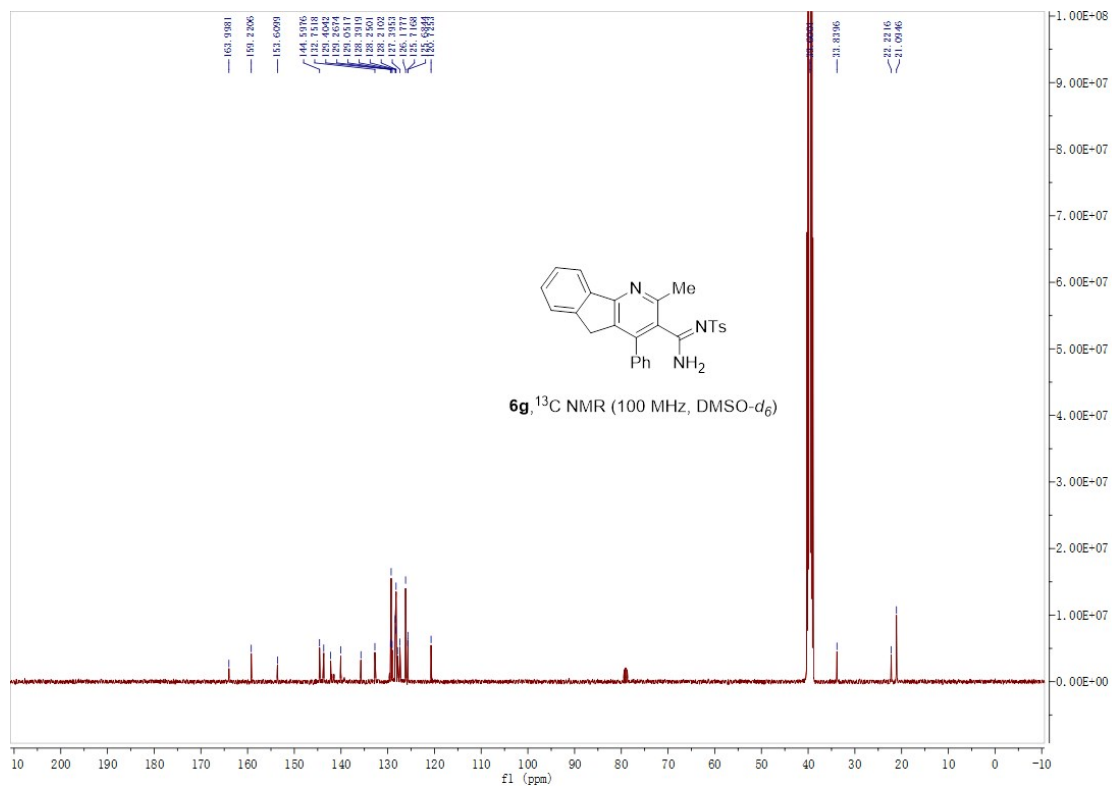
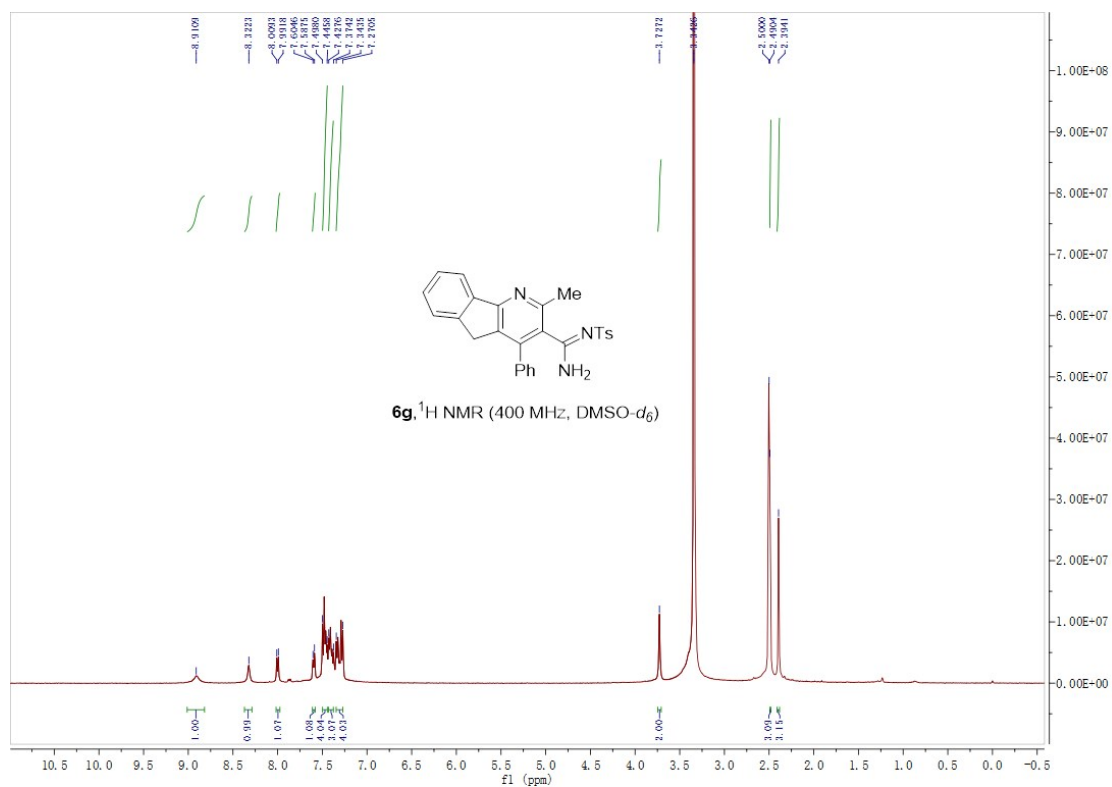


Figure S7. ^1H NMR of **6g** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6g** (100 MHz, $\text{DMSO-}d_6$).

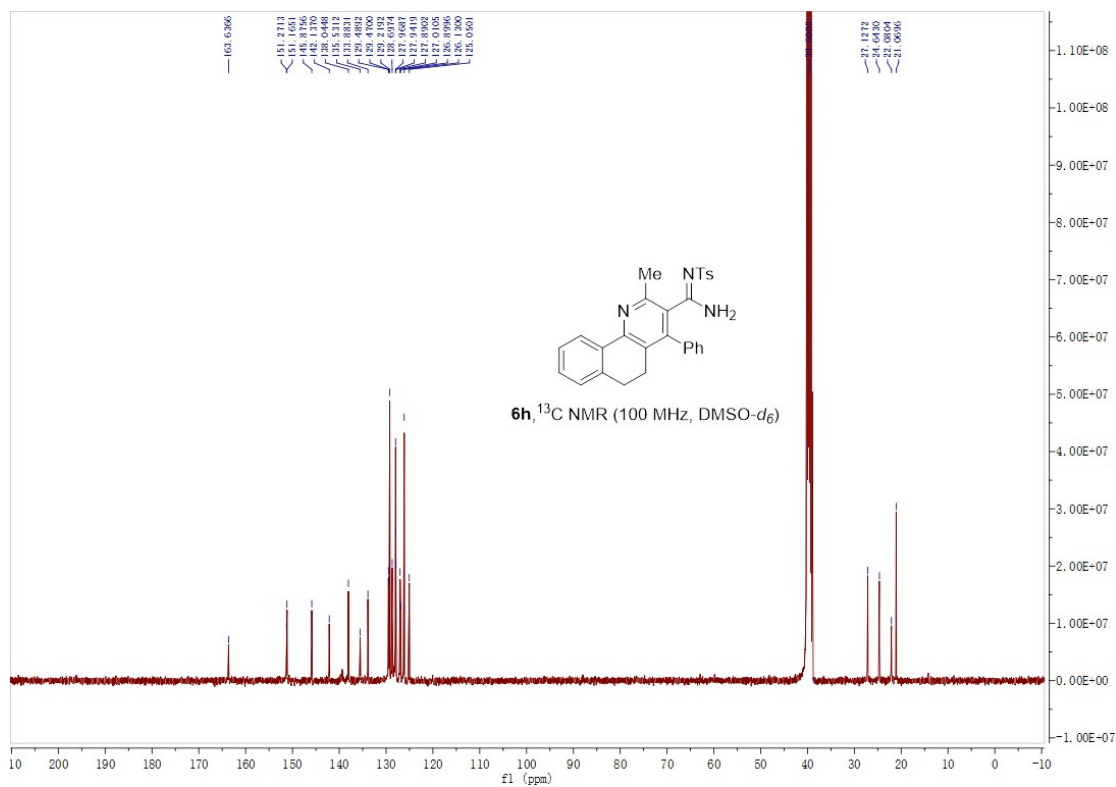
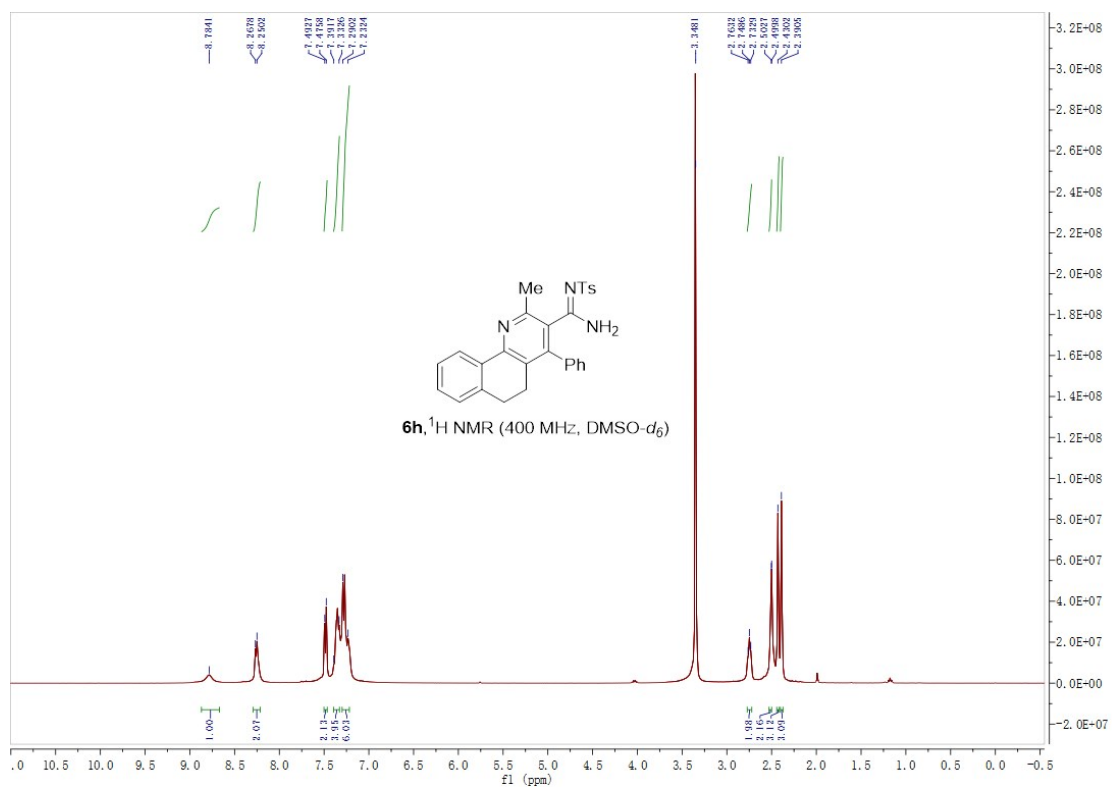


Figure S8. ^1H NMR of **6h** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6h** (100 MHz, $\text{DMSO-}d_6$).

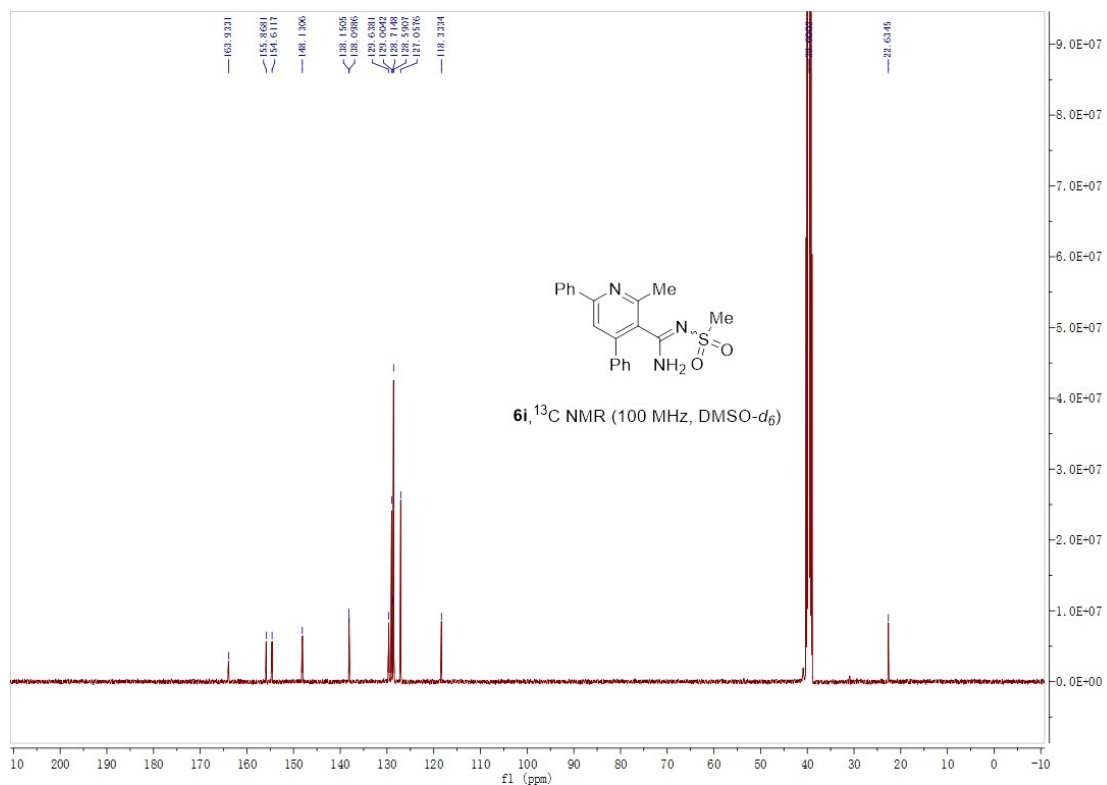
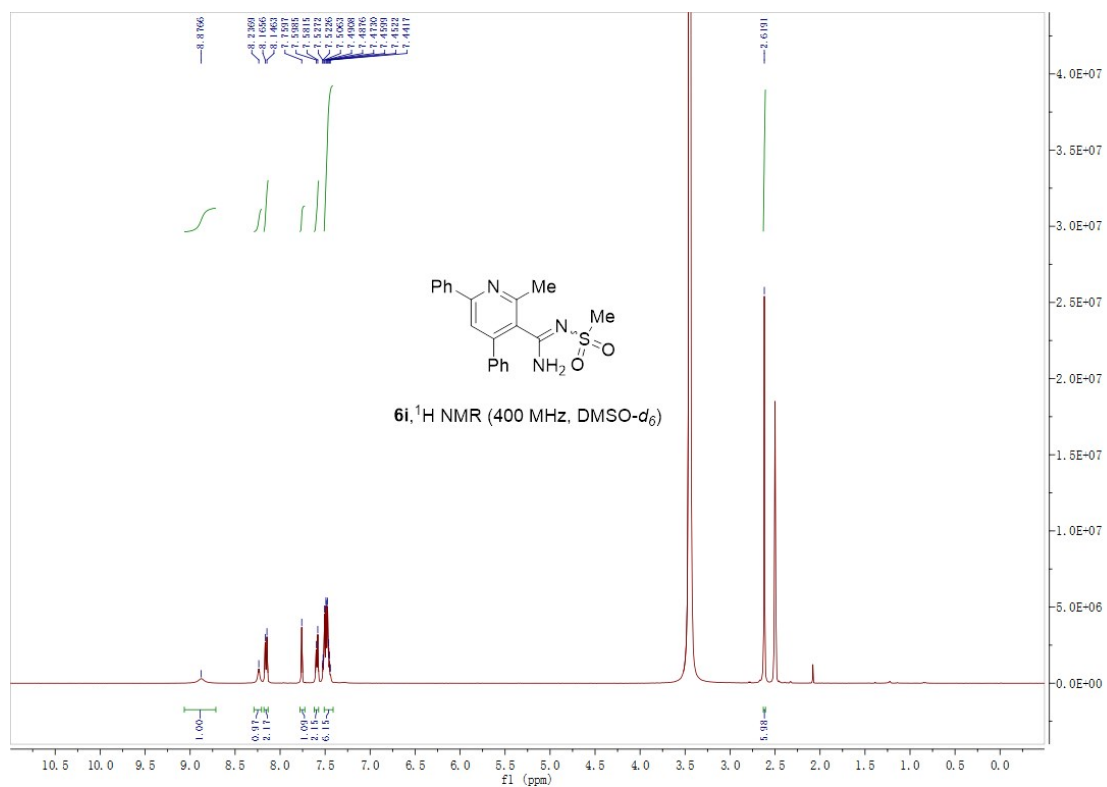


Figure S9. ^1H NMR of **6i** (400 MHz, $\text{DMSO}-d_6$) and ^{13}C NMR of **6i** (100 MHz, $\text{DMSO}-d_6$).

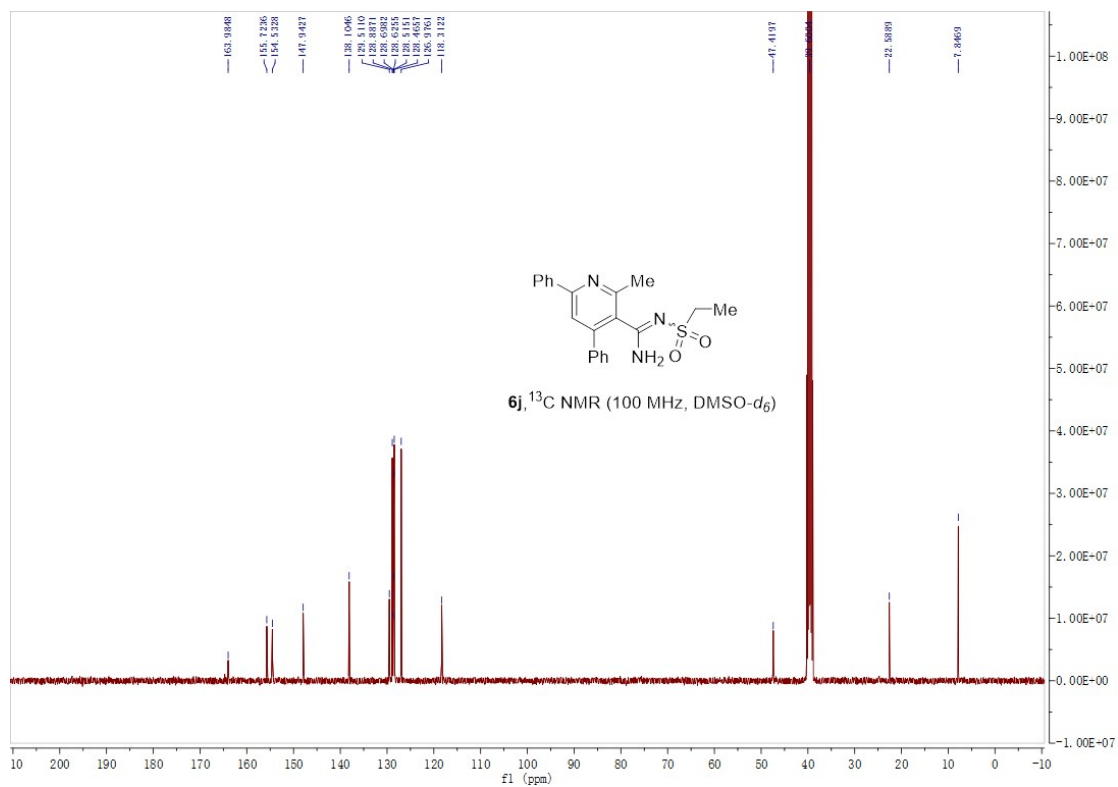
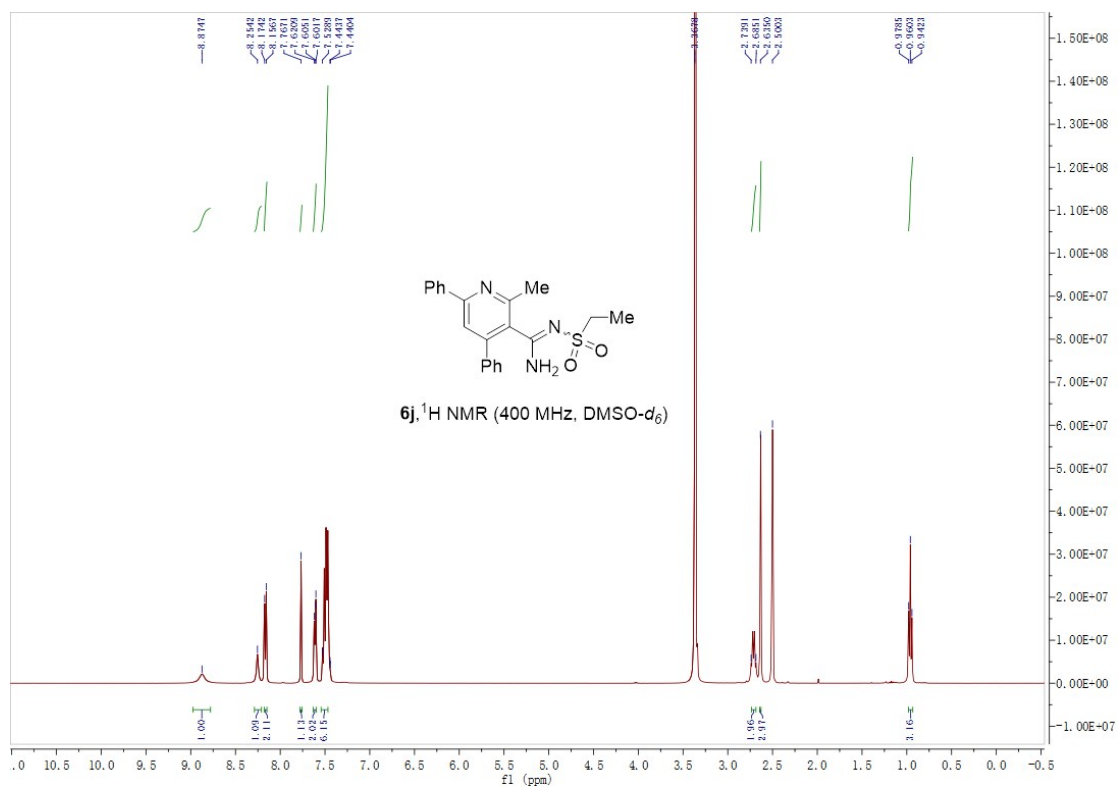


Figure S10. ^1H NMR of **6j** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6j** (100 MHz, $\text{DMSO-}d_6$).

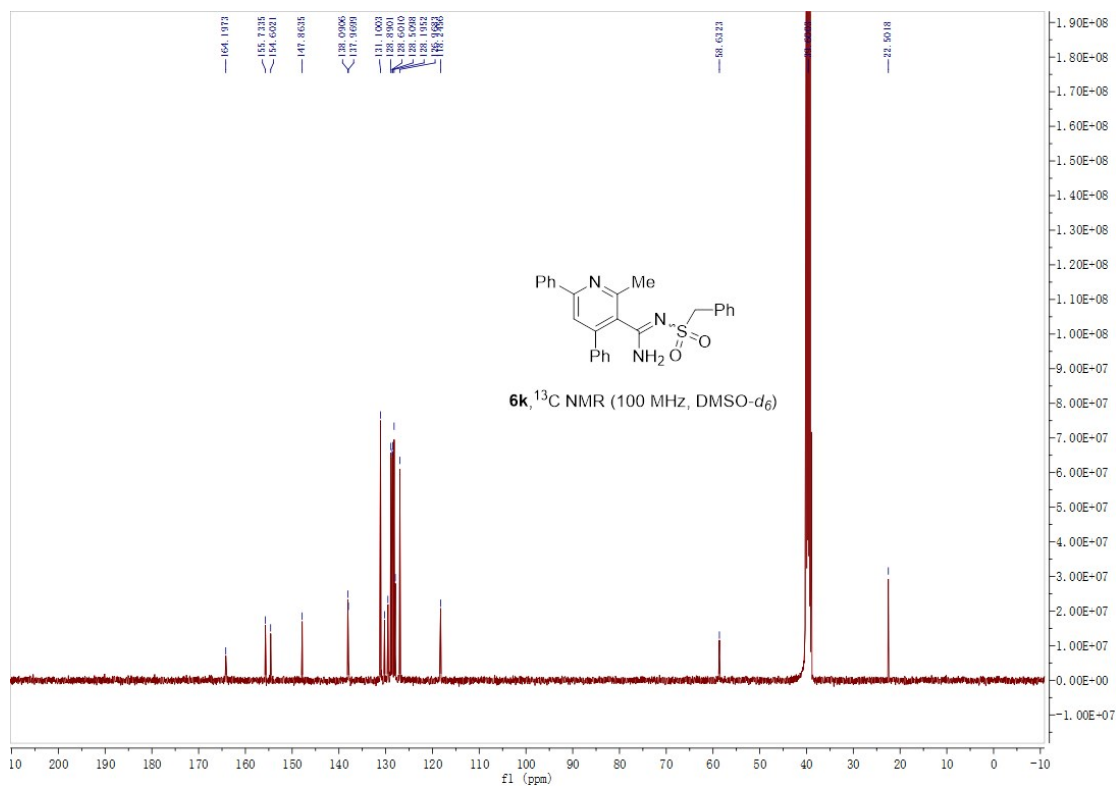
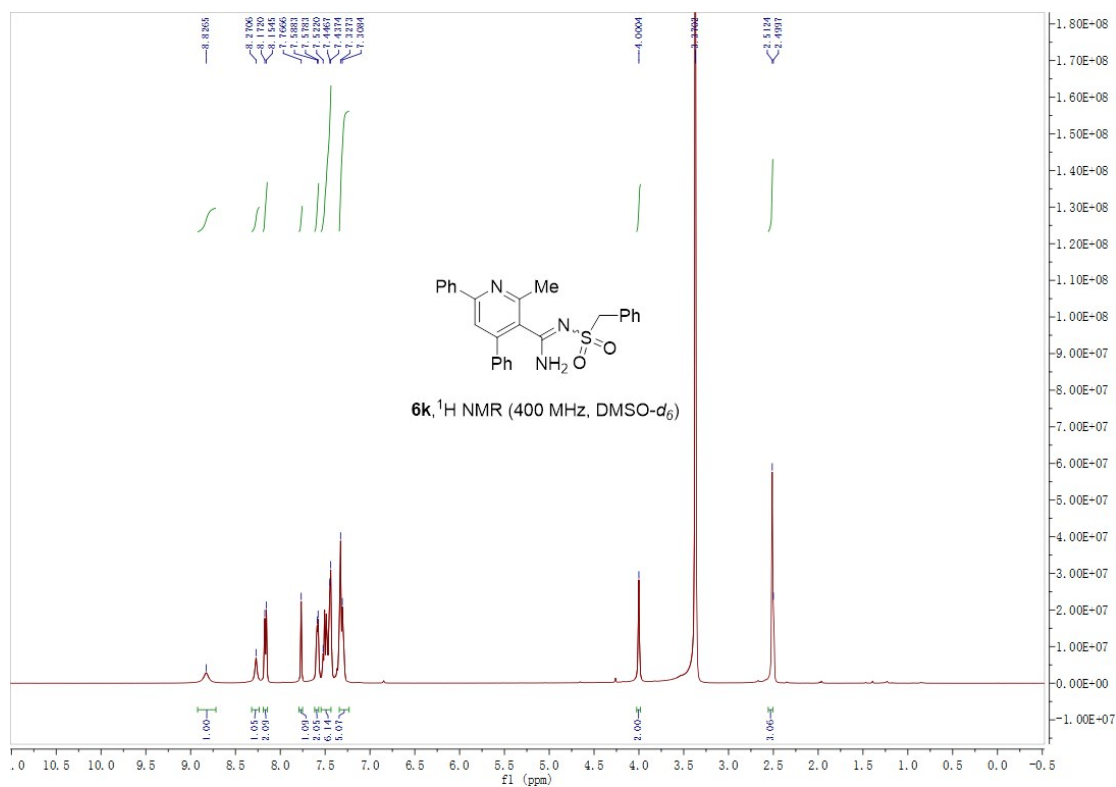


Figure S11. ^1H NMR of **6k** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6k** (100 MHz, $\text{DMSO-}d_6$).

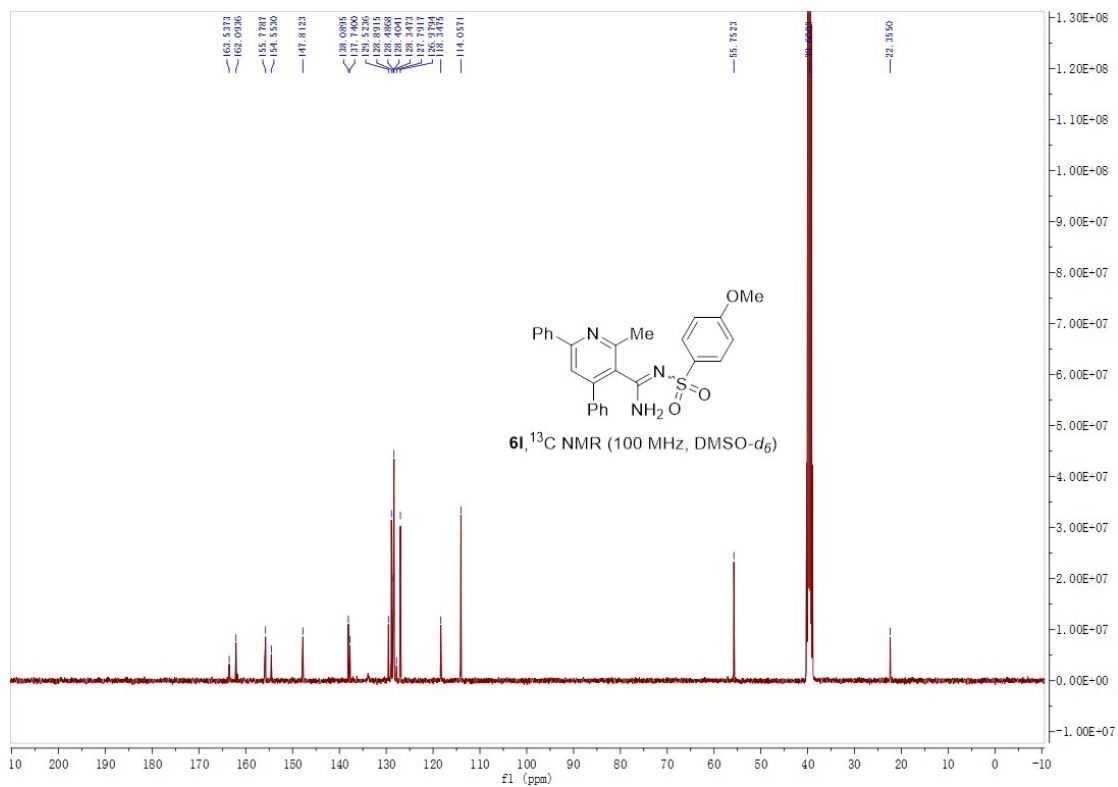
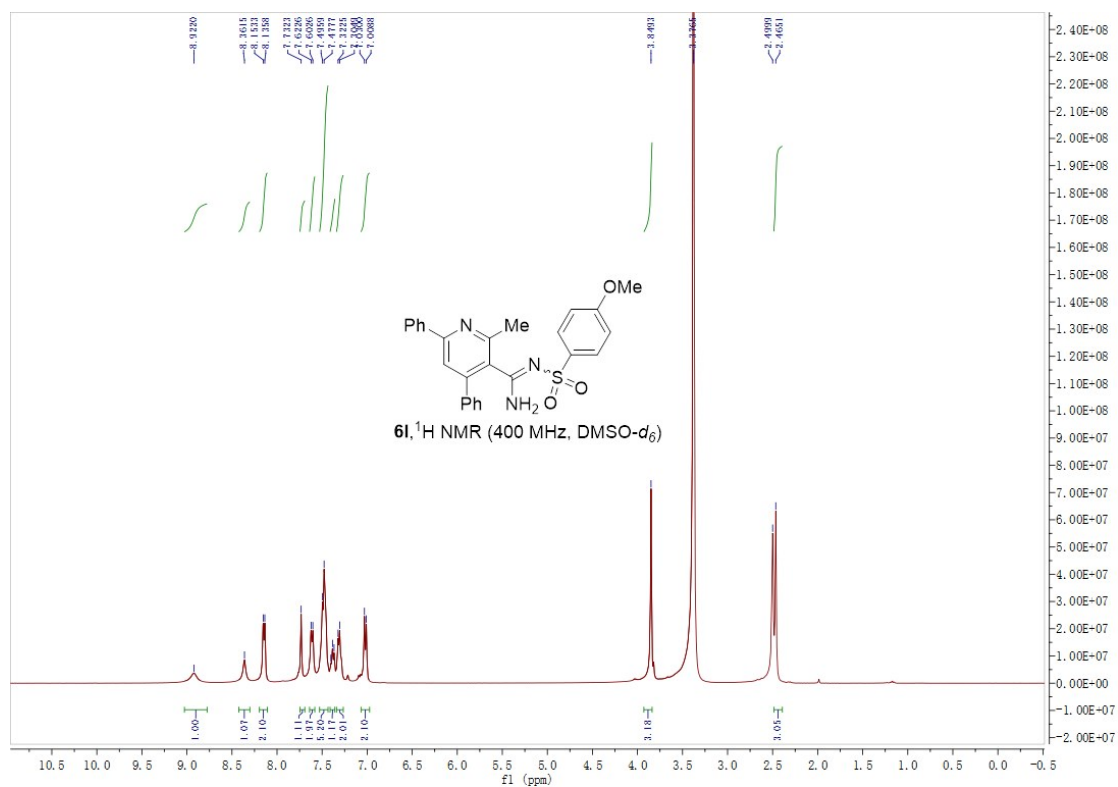


Figure S12. ¹H NMR of **6l** (400 MHz, DMSO-*d*₆) and ¹³C NMR of **6l** (100 MHz, DMSO-*d*₆).

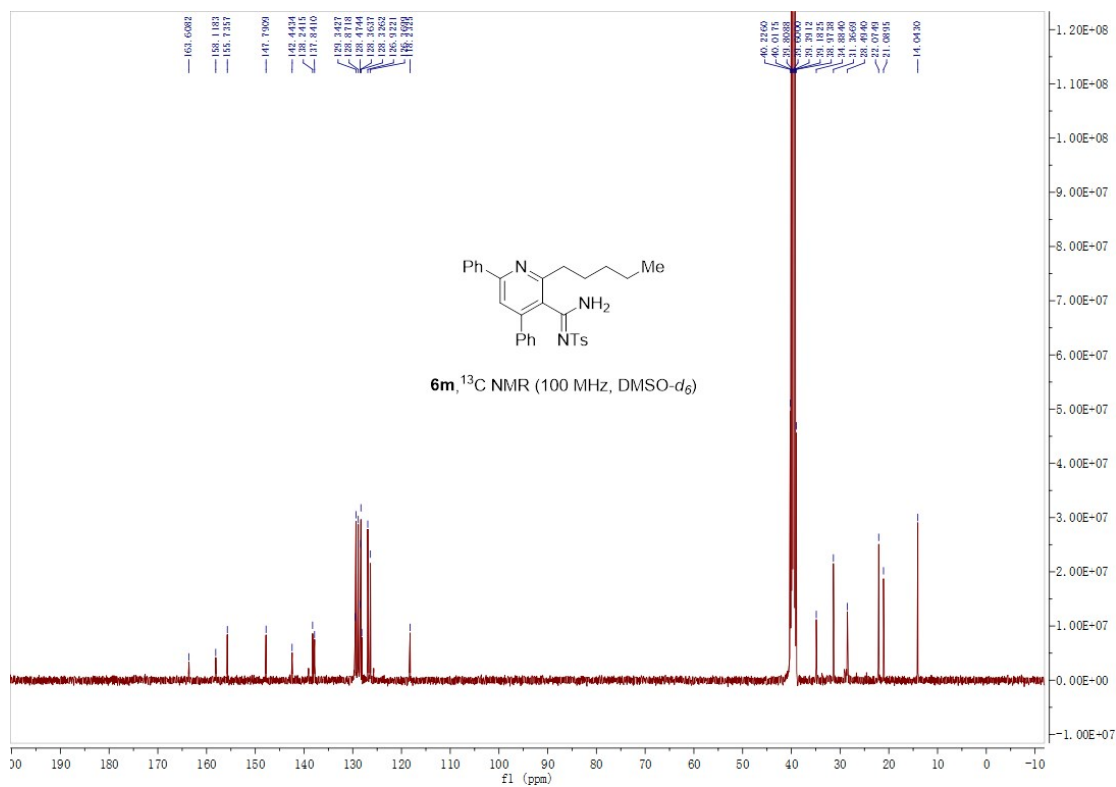
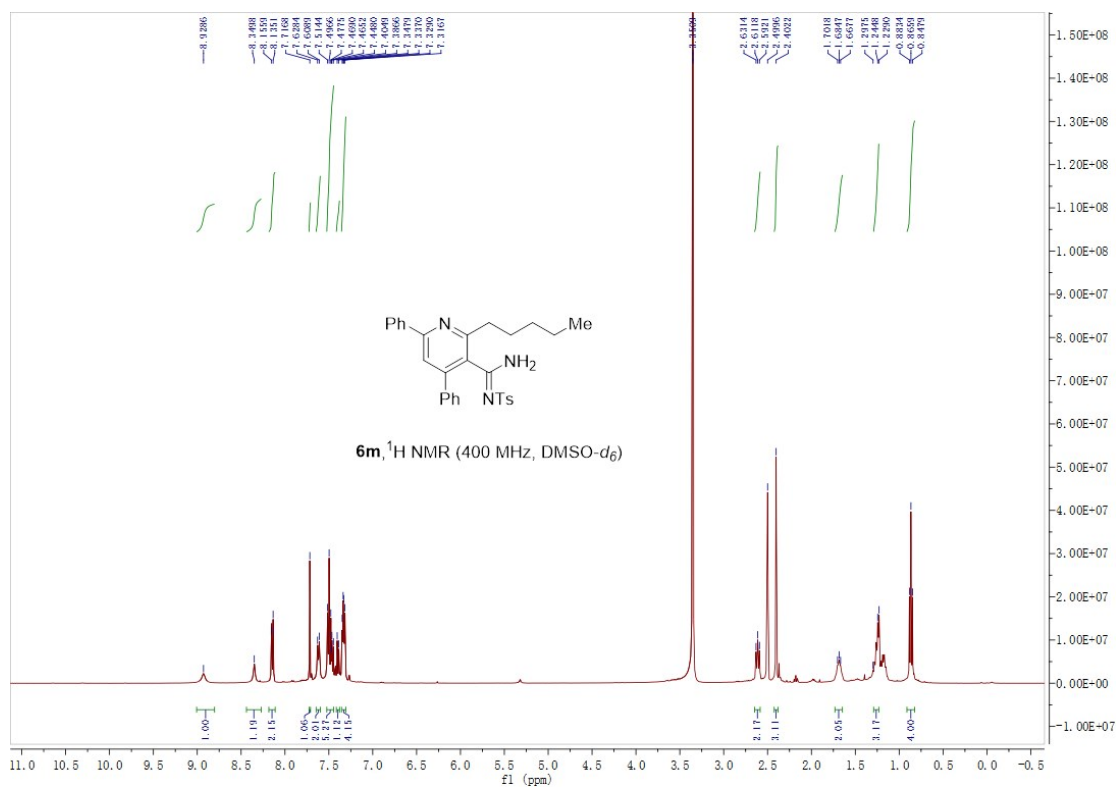


Figure S13. ^1H NMR of **6m** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6m** (100 MHz, $\text{DMSO-}d_6$).

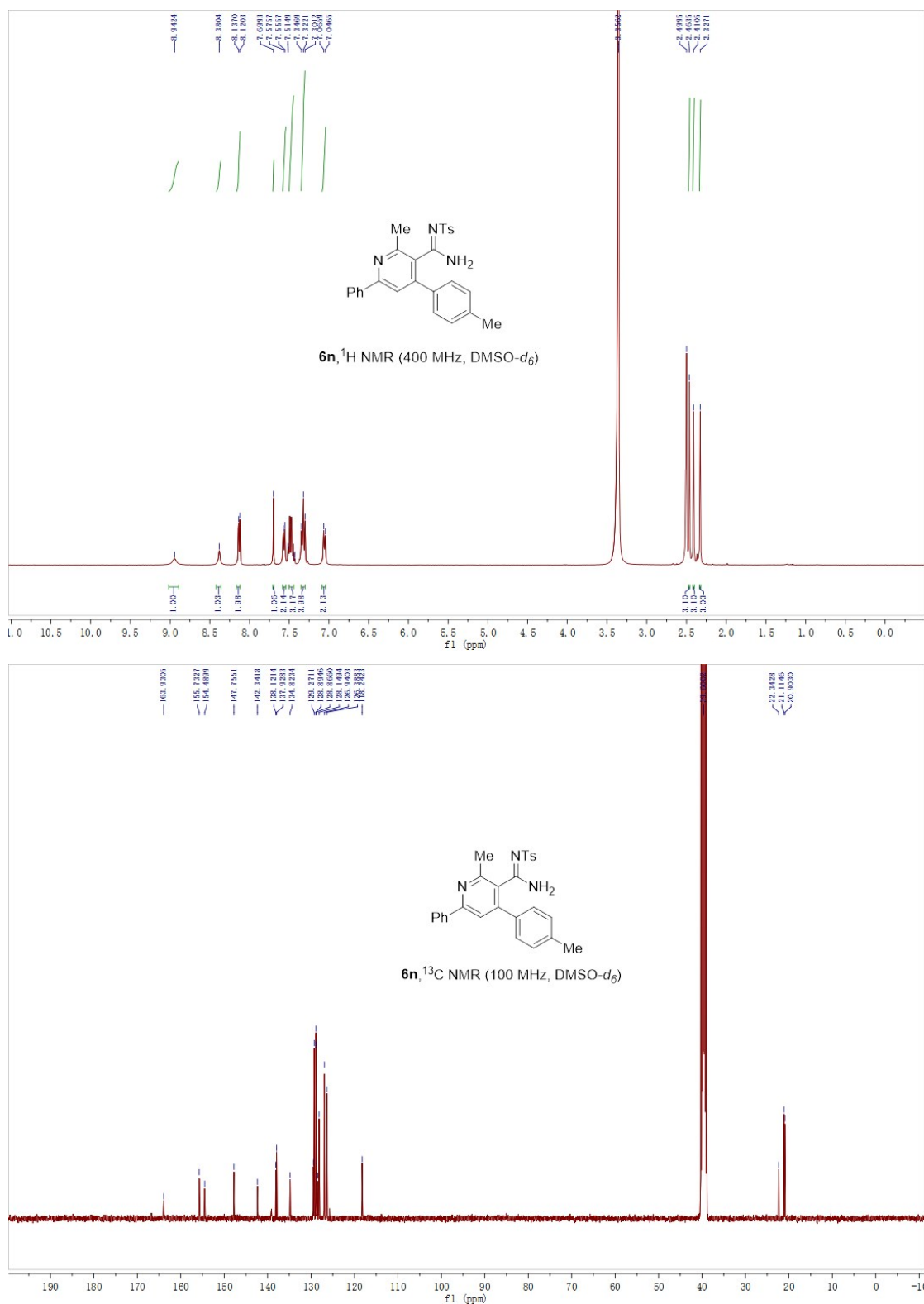


Figure S14. ^1H NMR of 6n (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of 6n (100 MHz, $\text{DMSO-}d_6$).

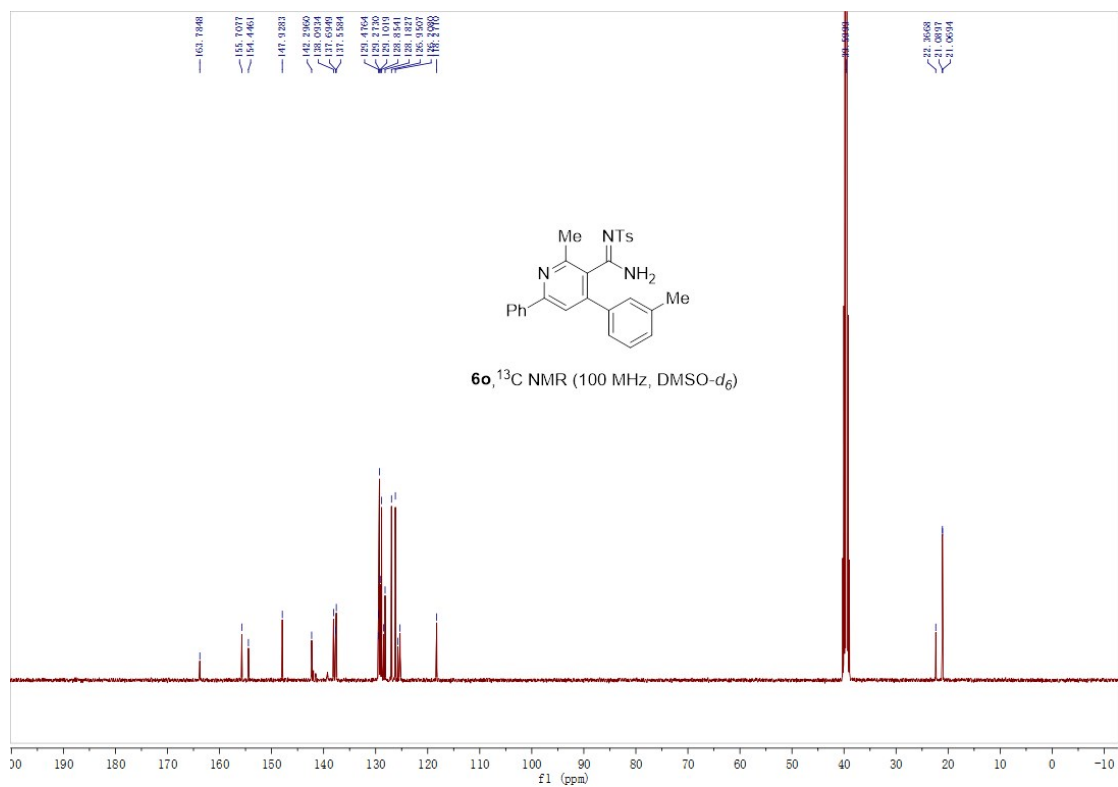
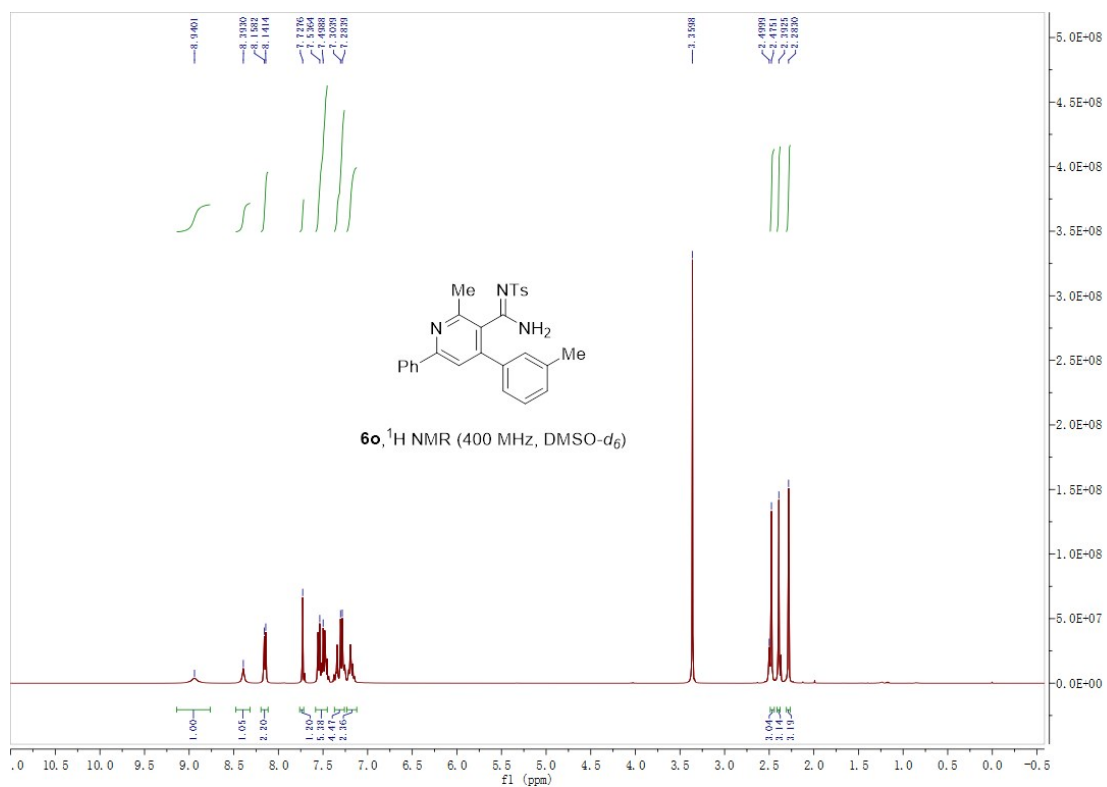


Figure S15. ^1H NMR of **6o** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6o** (100 MHz, $\text{DMSO-}d_6$).

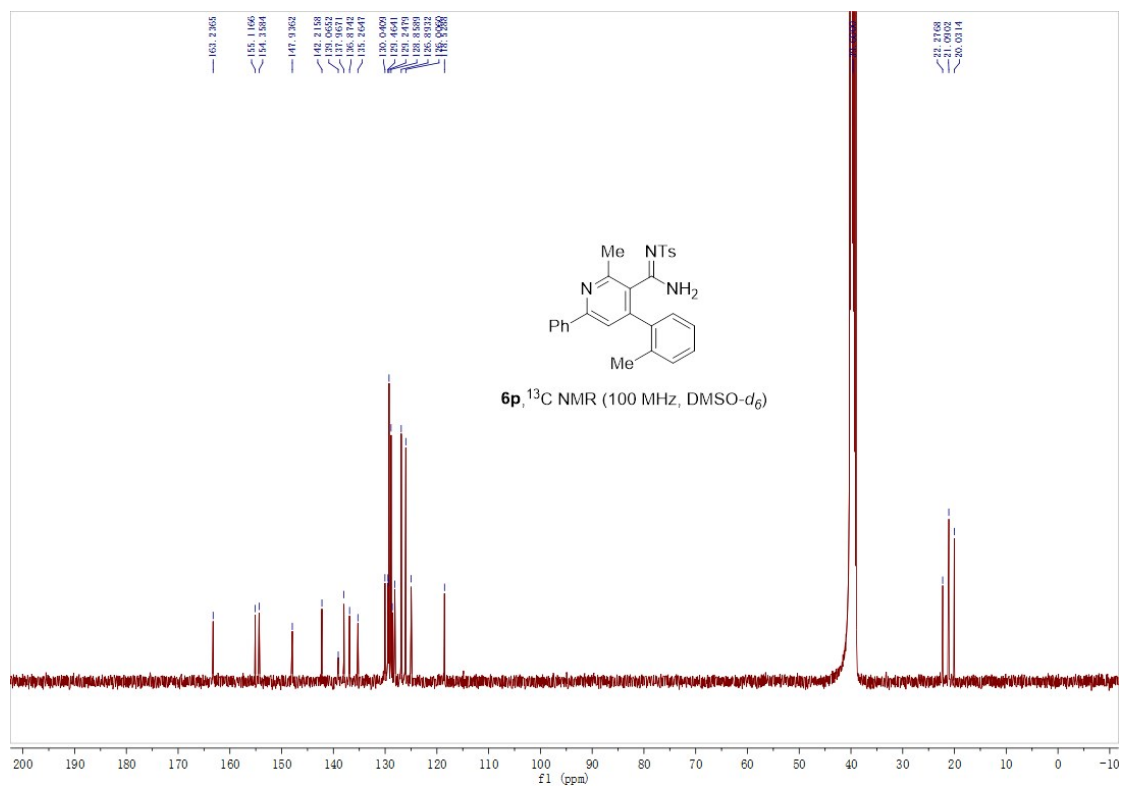
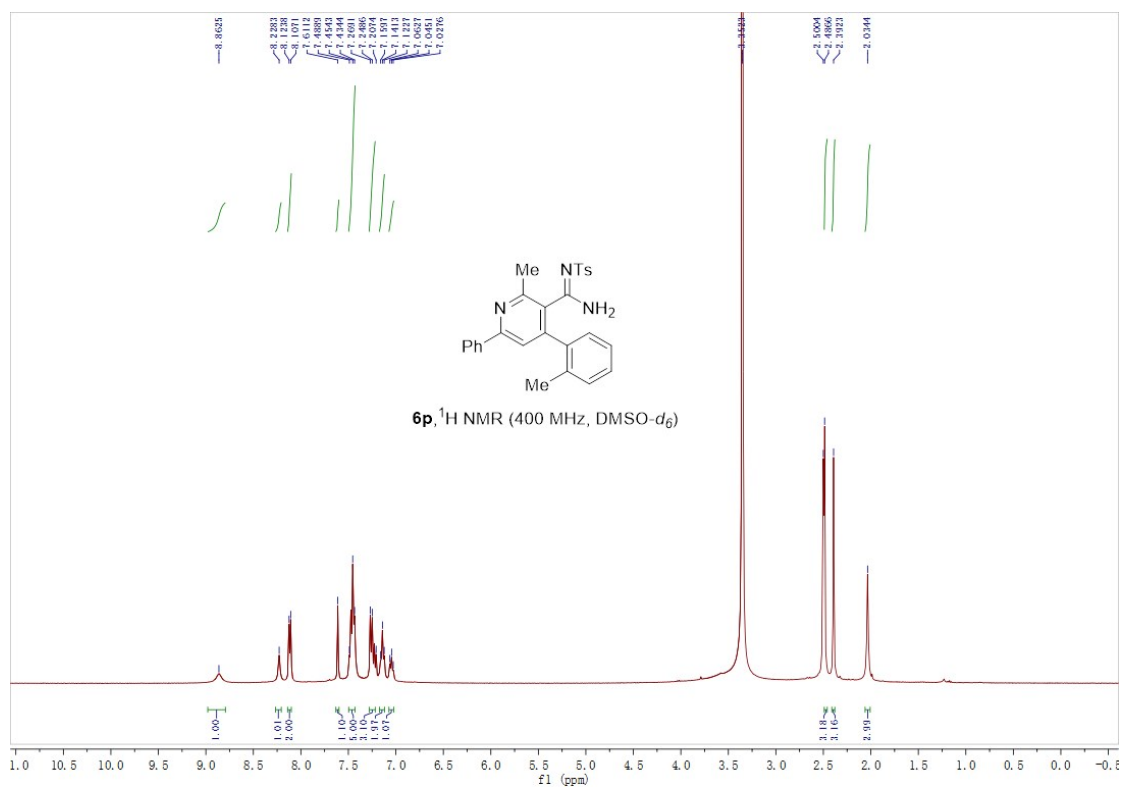


Figure S16. ^1H NMR of **6p** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6p** (100 MHz, $\text{DMSO-}d_6$).

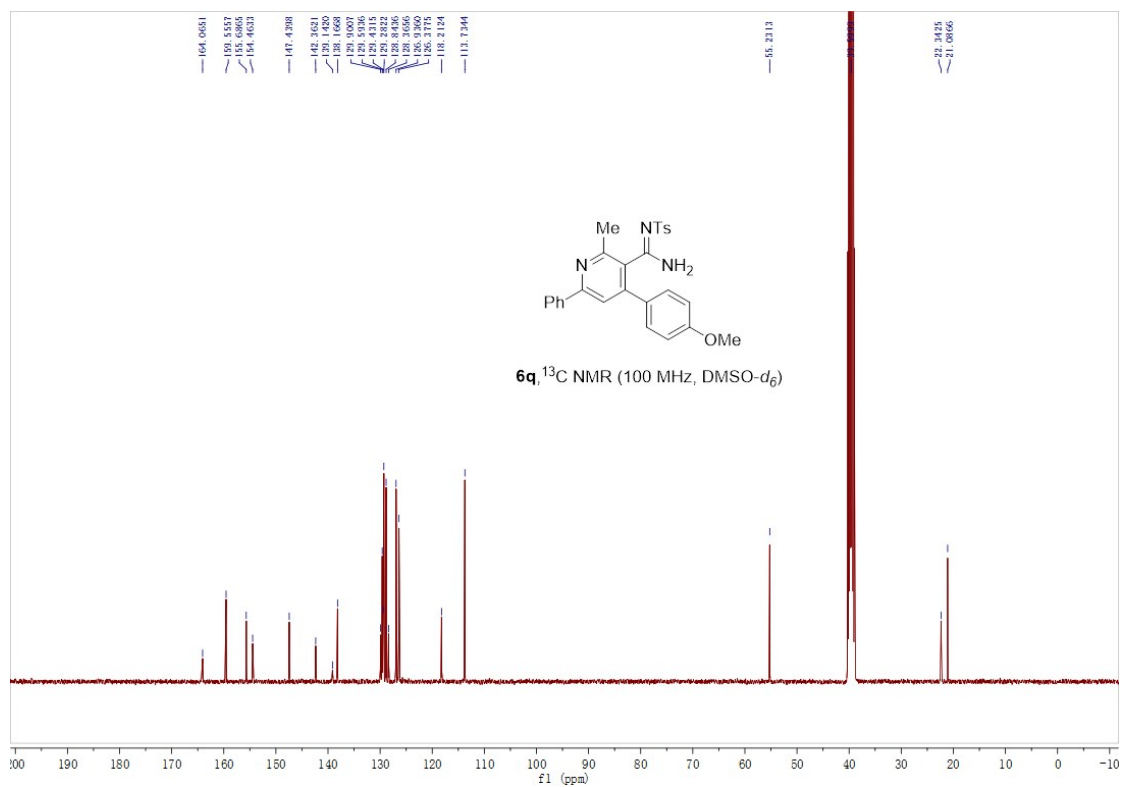
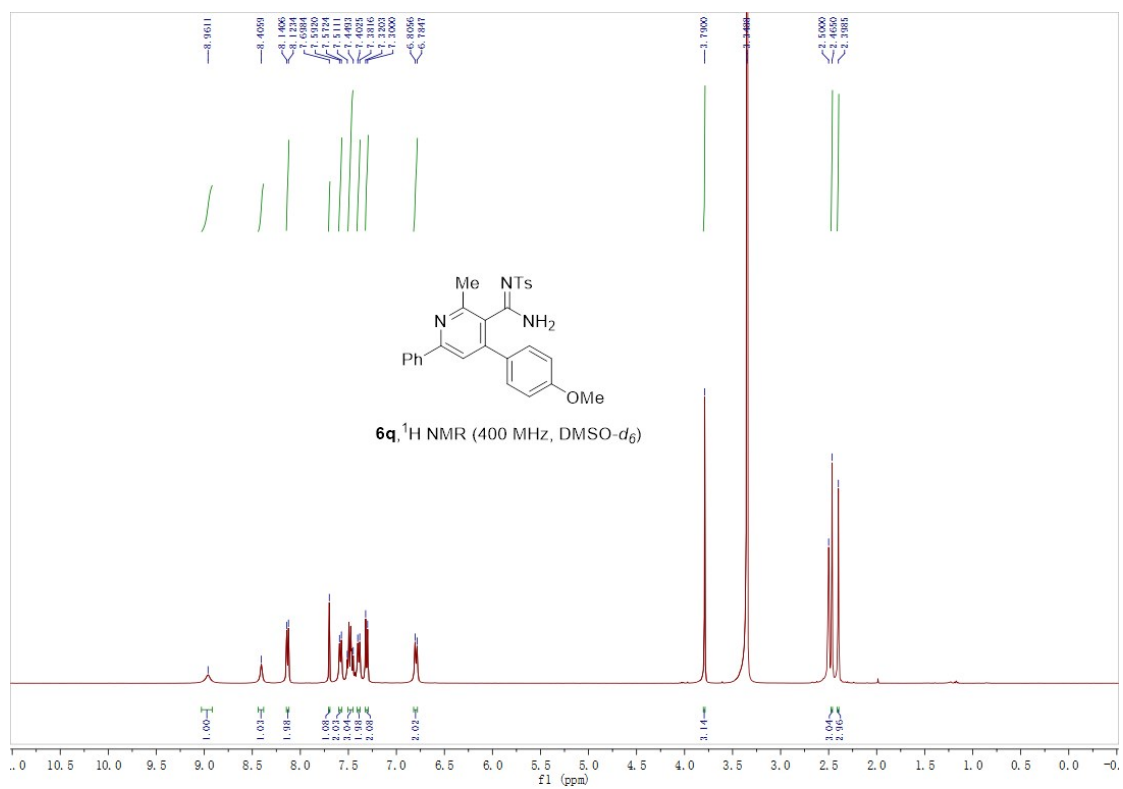


Figure S17. ¹H NMR of **6q** (400 MHz, DMSO-*d*₆) and ¹³C NMR of **6q** (100 MHz, DMSO-*d*₆).

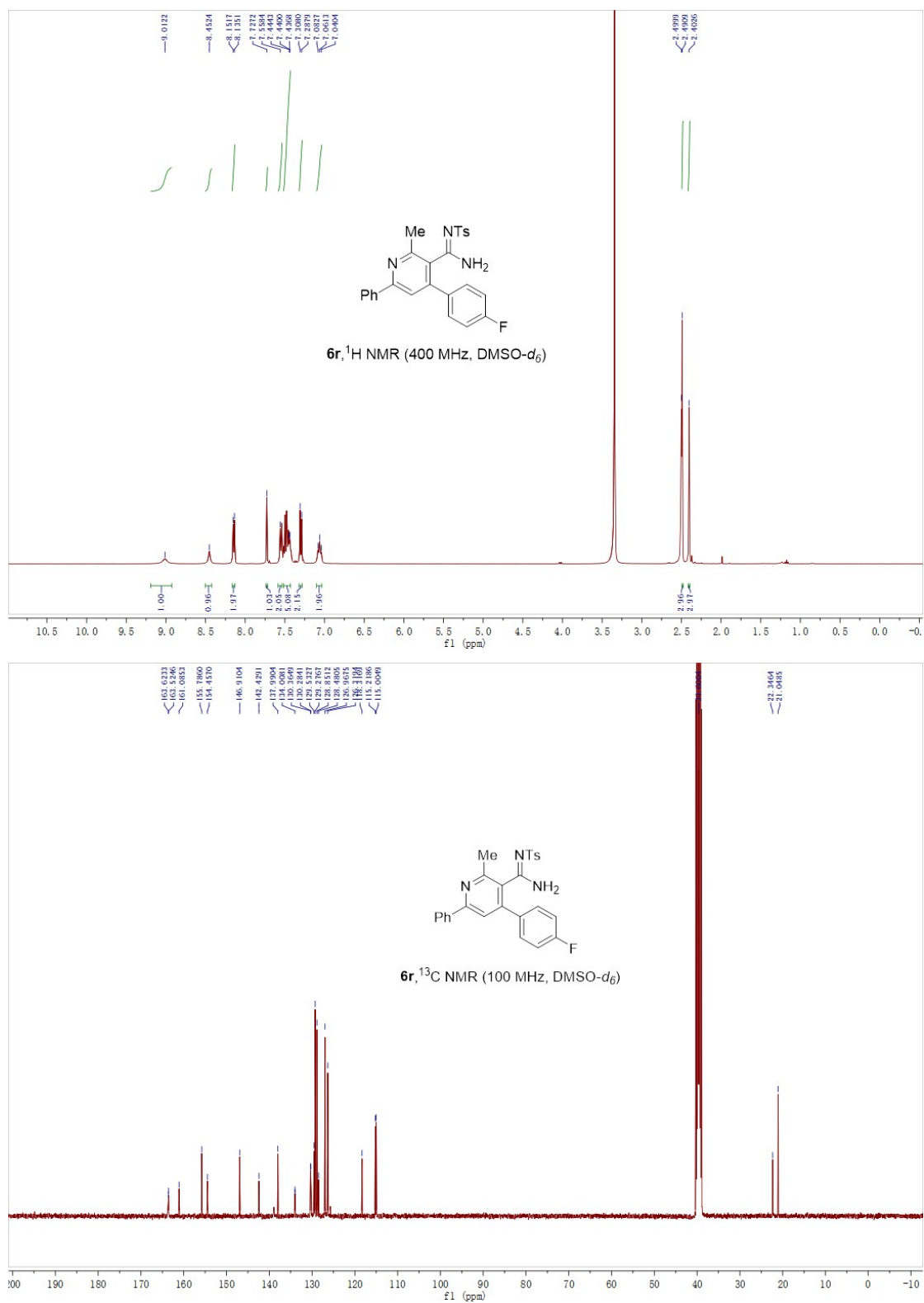


Figure S18. ^1H NMR of **6r** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6r** (100 MHz, $\text{DMSO-}d_6$).

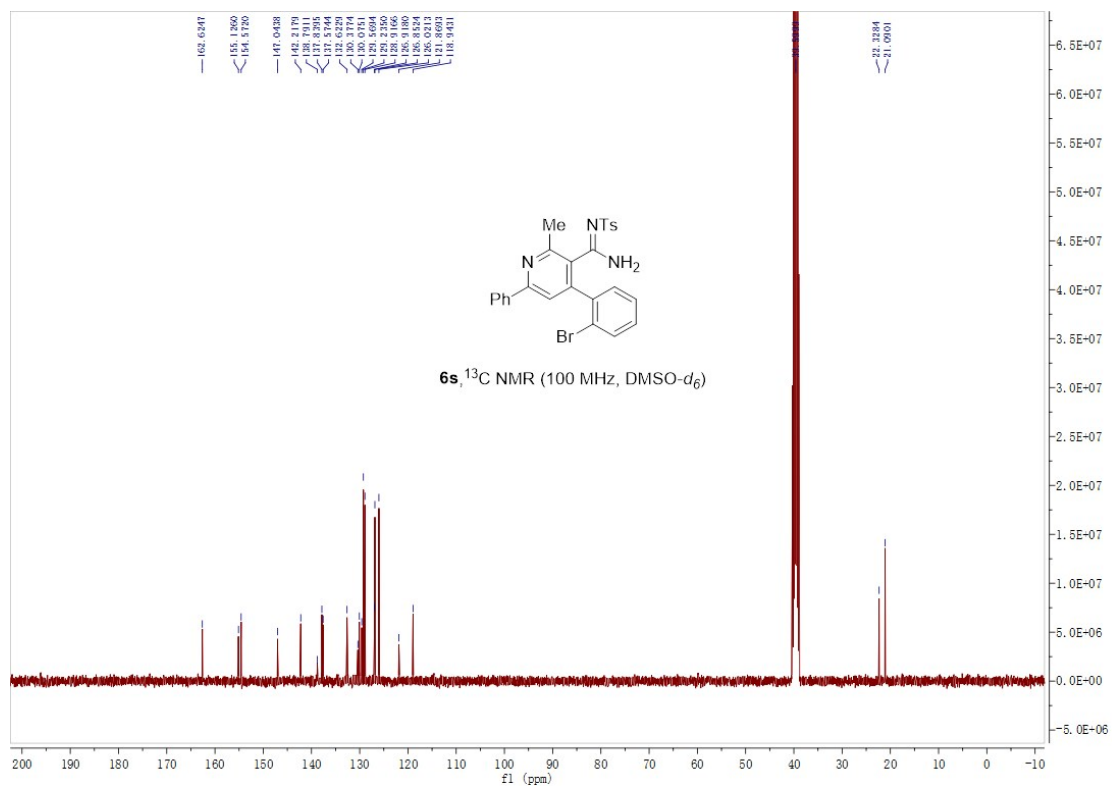
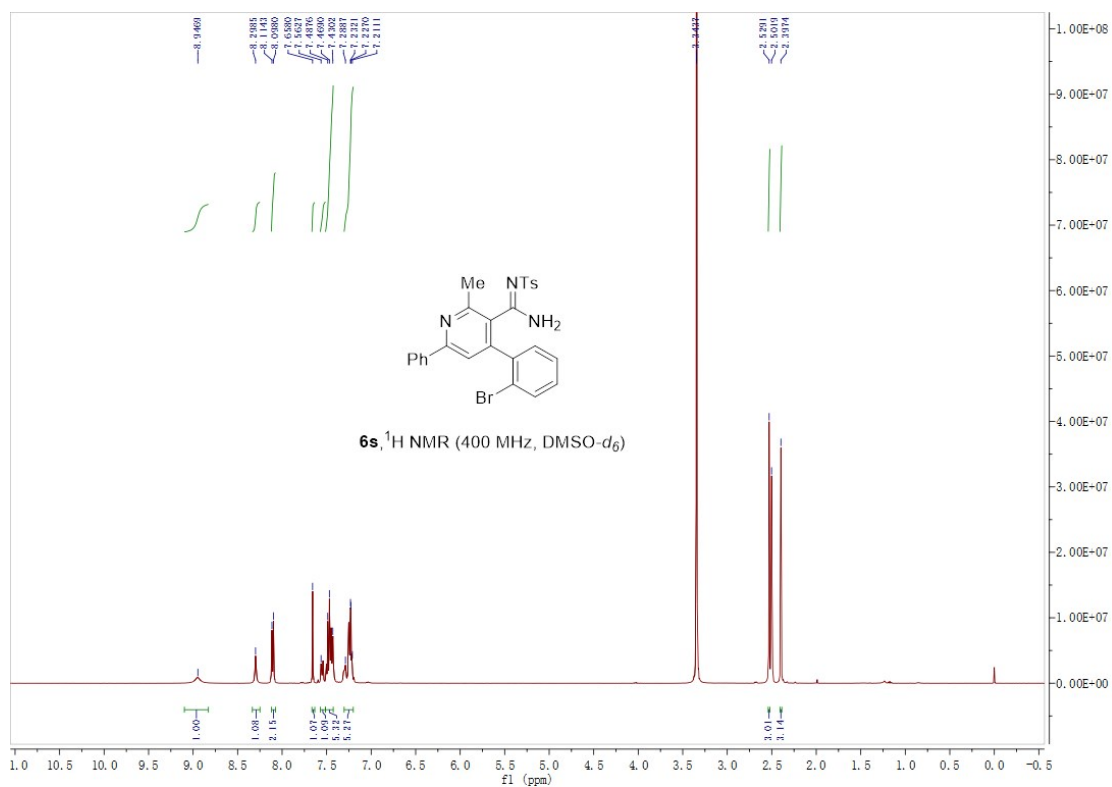


Figure S19. ^1H NMR of **6s** (400 MHz, $\text{DMSO}-d_6$) and ^{13}C NMR of **6s** (100 MHz, $\text{DMSO}-d_6$).

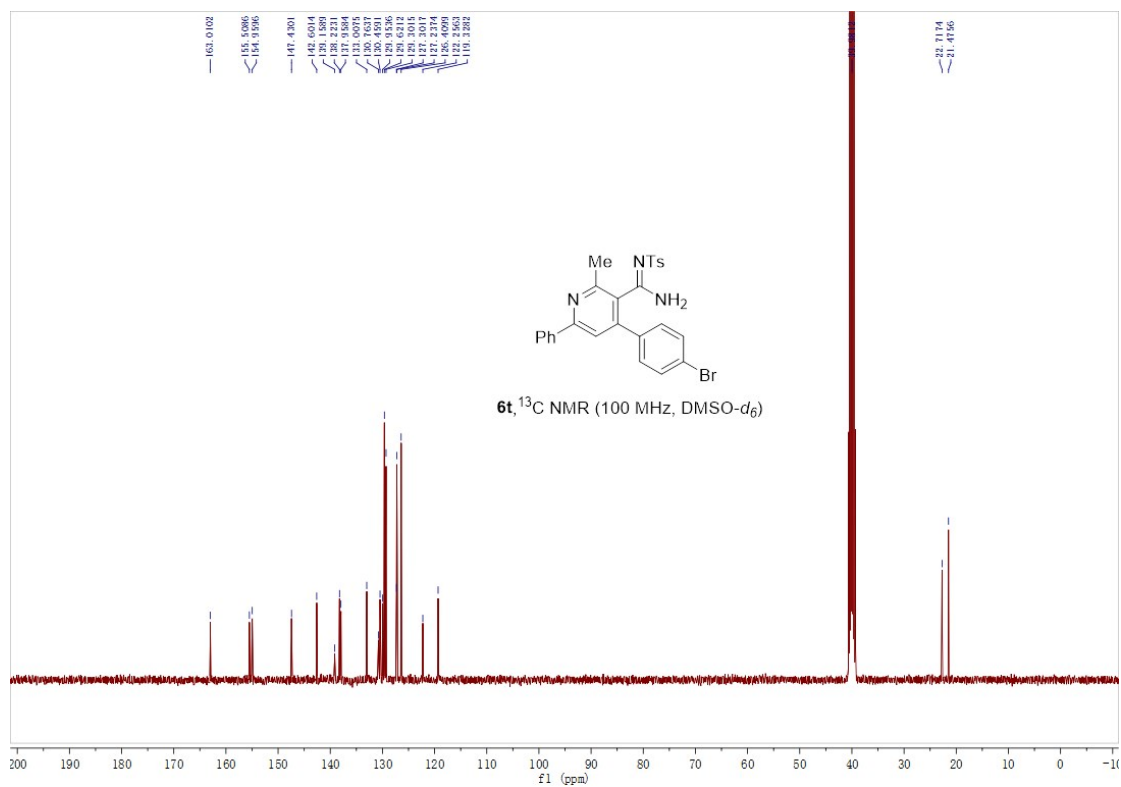
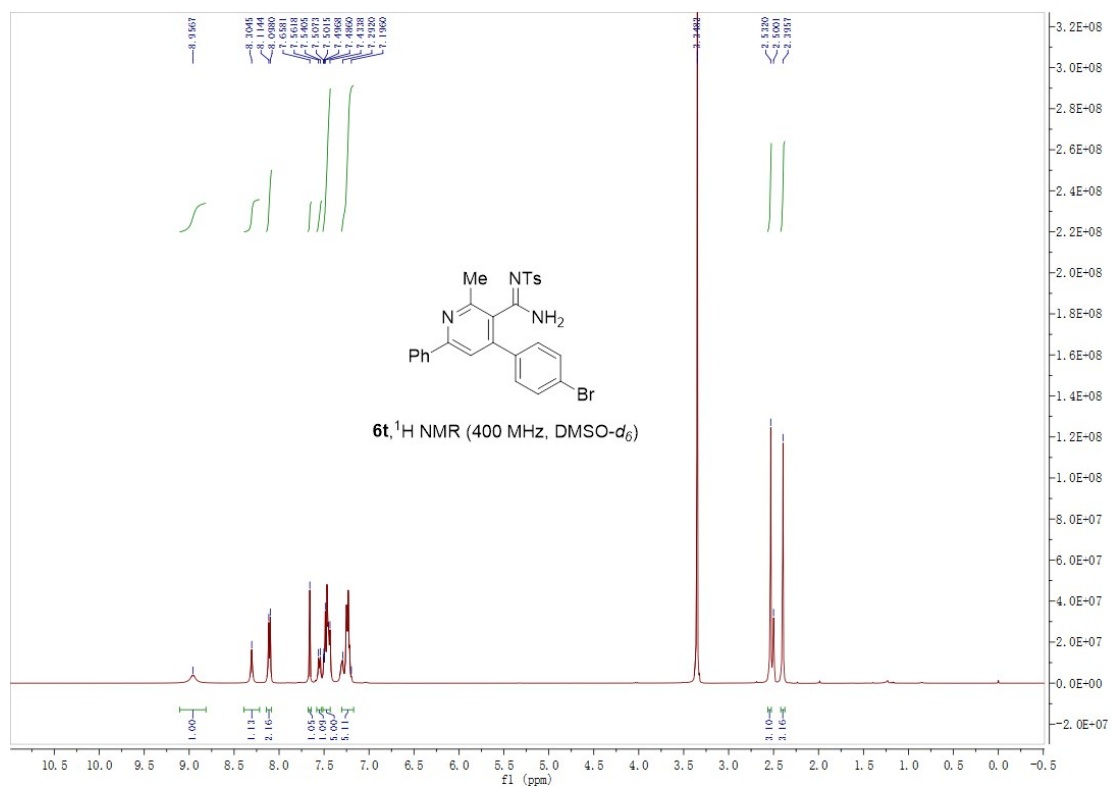


Figure S20. ^1H NMR of **6t** (400 MHz, $\text{DMSO}-d_6$) and ^{13}C NMR of **6t** (100 MHz, $\text{DMSO}-d_6$).

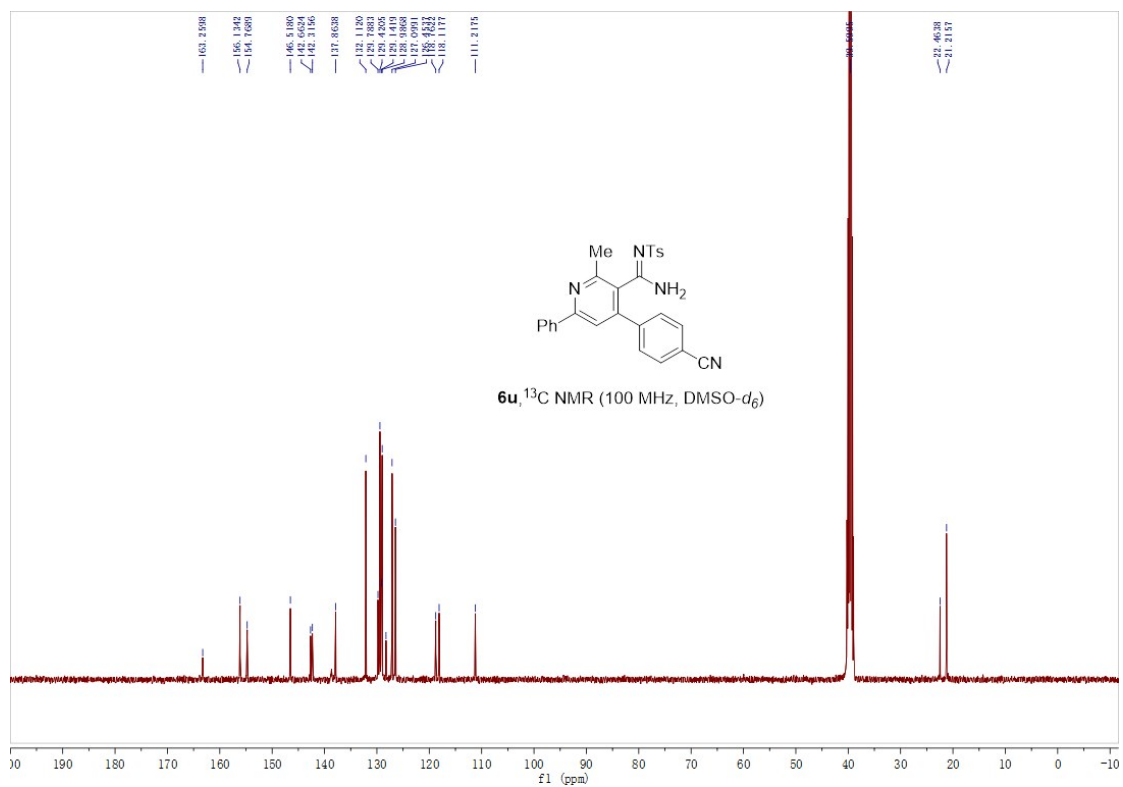
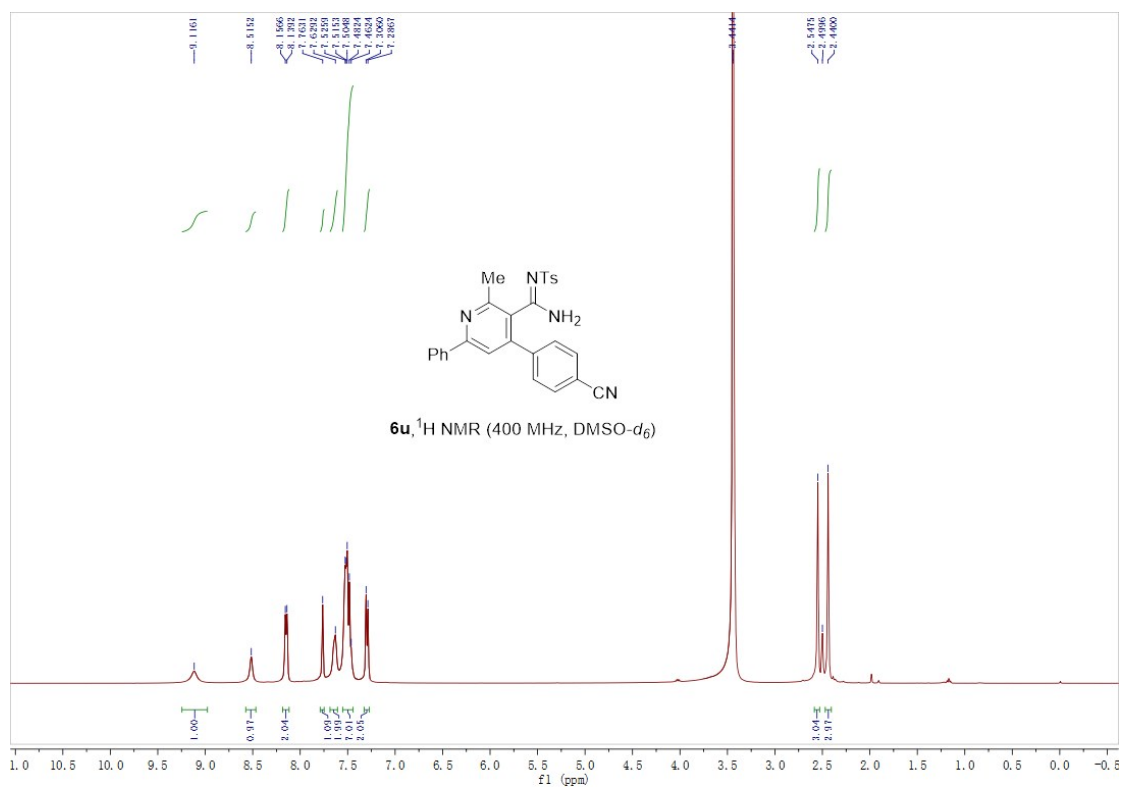


Figure S21. ^1H NMR of **6u** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6u** (100 MHz, $\text{DMSO-}d_6$).

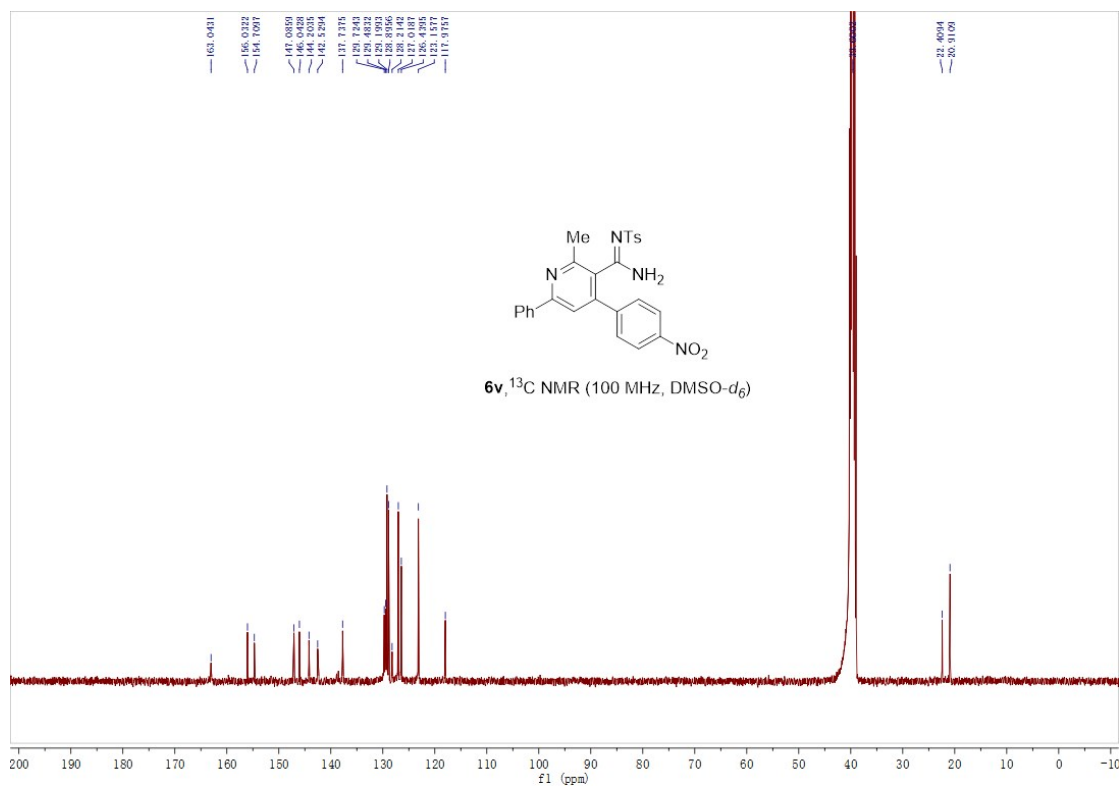
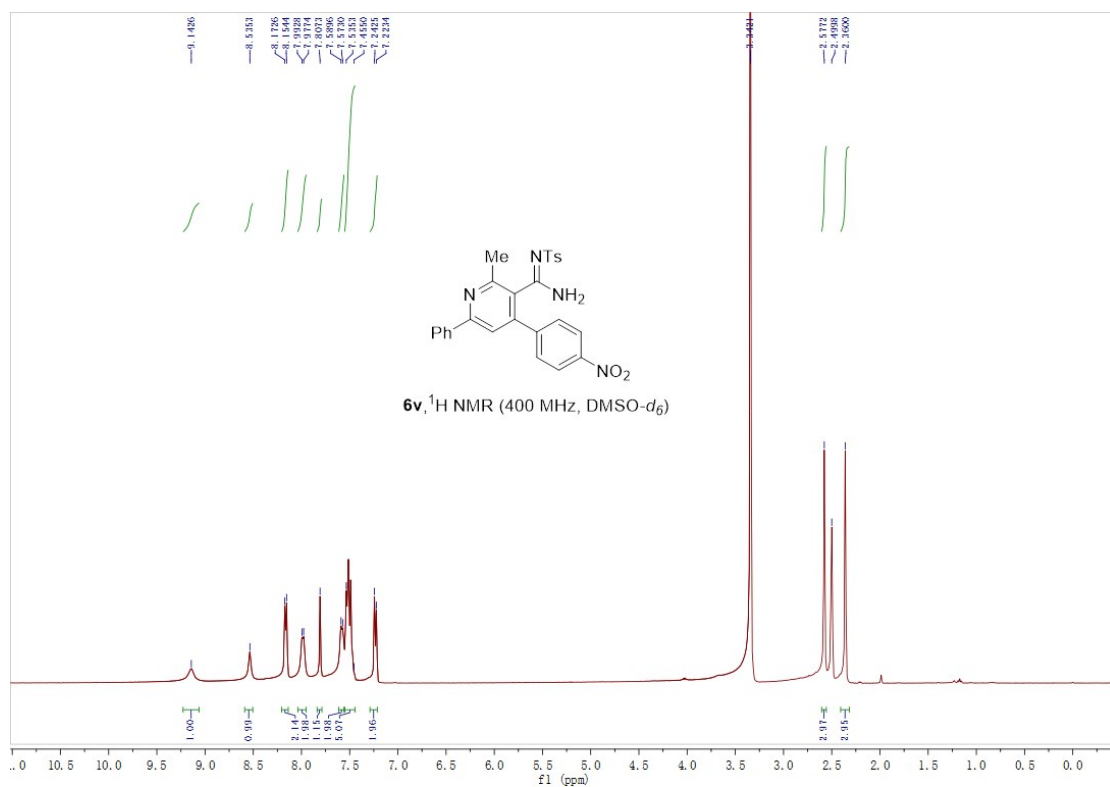


Figure S22. $^1\text{H NMR}$ of **6v** (400 MHz, $\text{DMSO-}d_6$) and $^{13}\text{C NMR}$ of **6v** (100 MHz, $\text{DMSO-}d_6$).

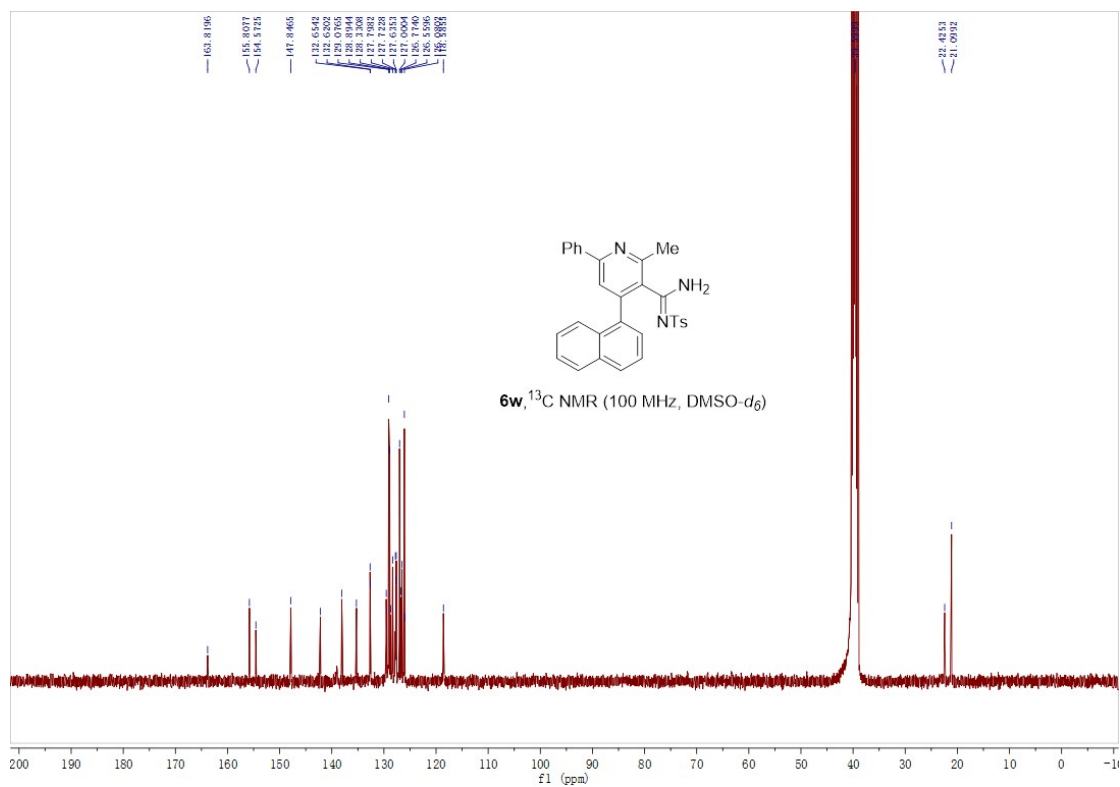
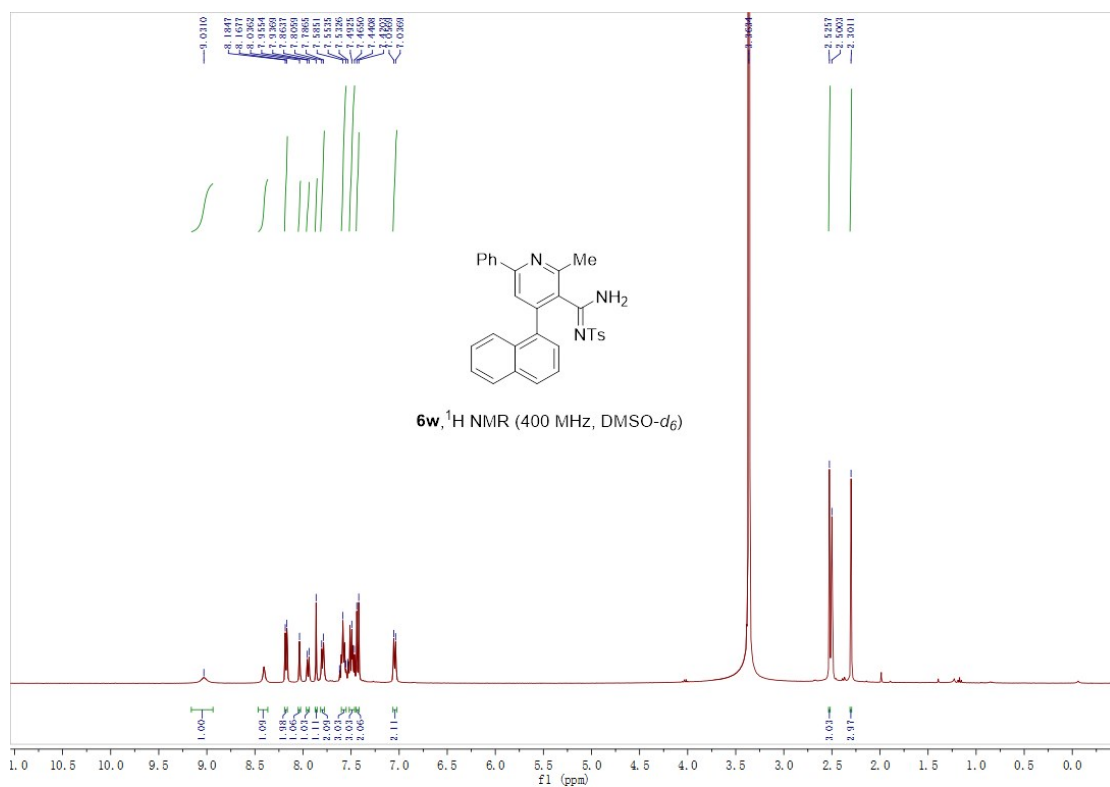


Figure S23. ^1H NMR of **6w** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6w** (100 MHz, $\text{DMSO-}d_6$).

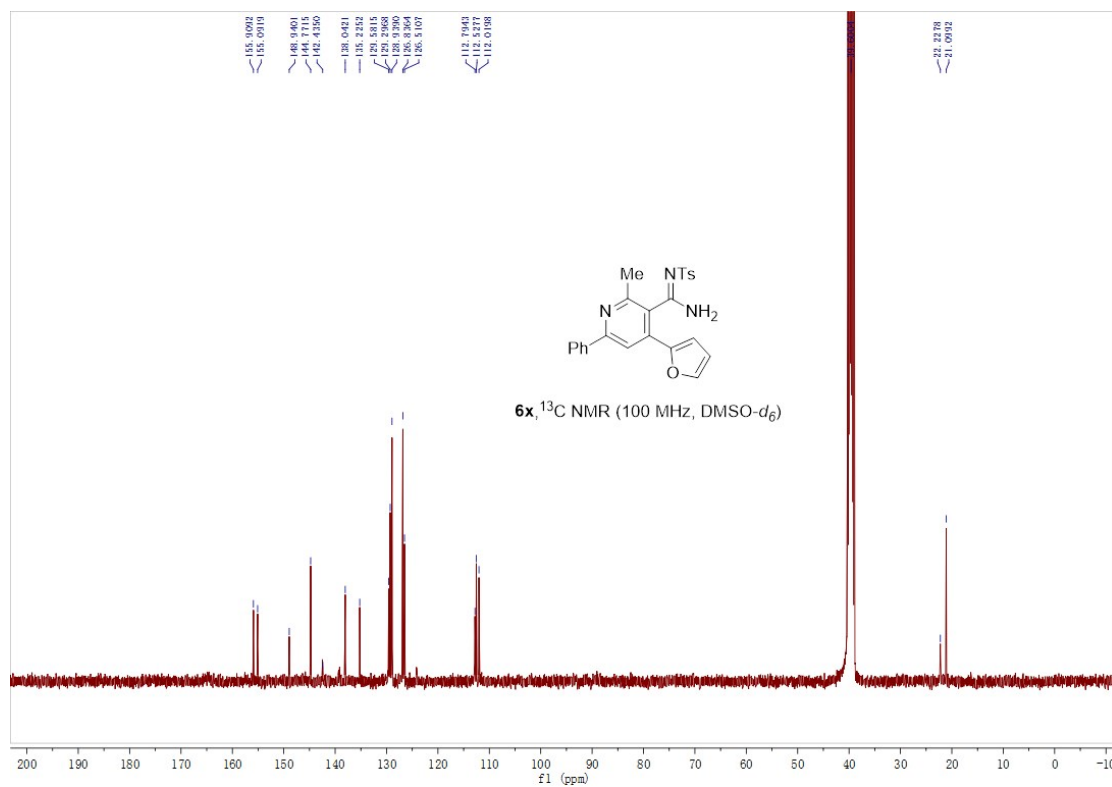
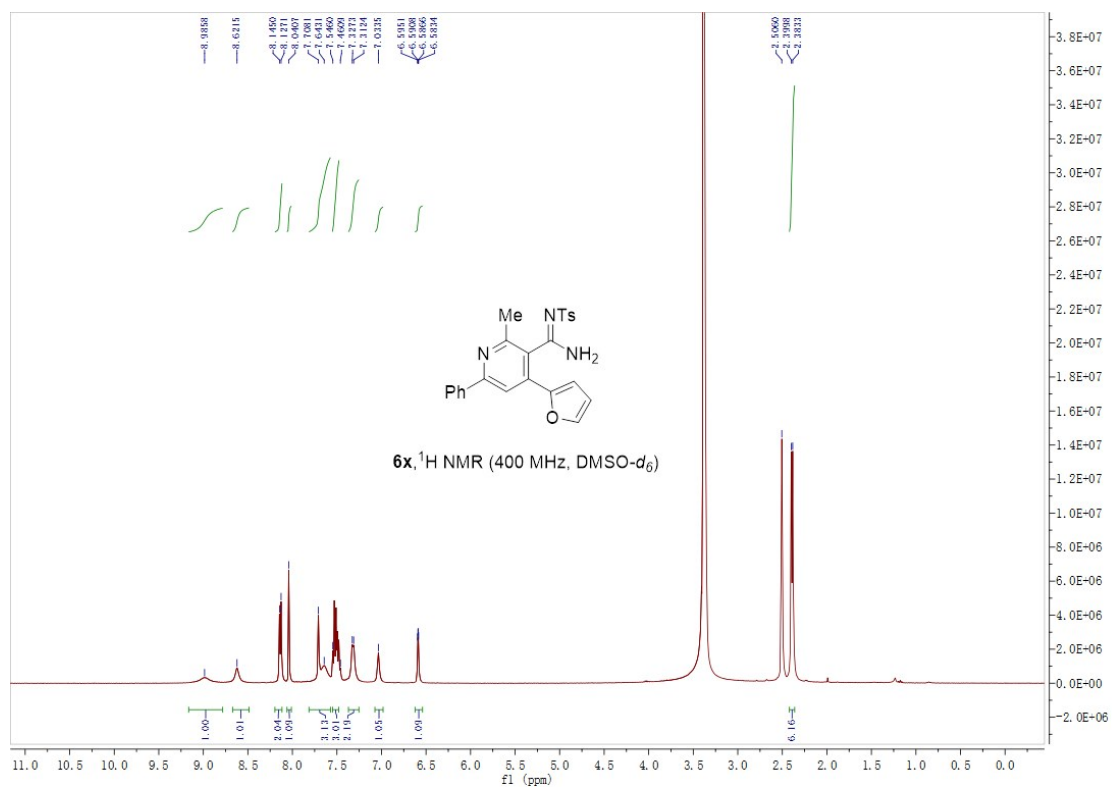


Figure S24. ^1H NMR of **6x** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6x** (100 MHz, $\text{DMSO-}d_6$).

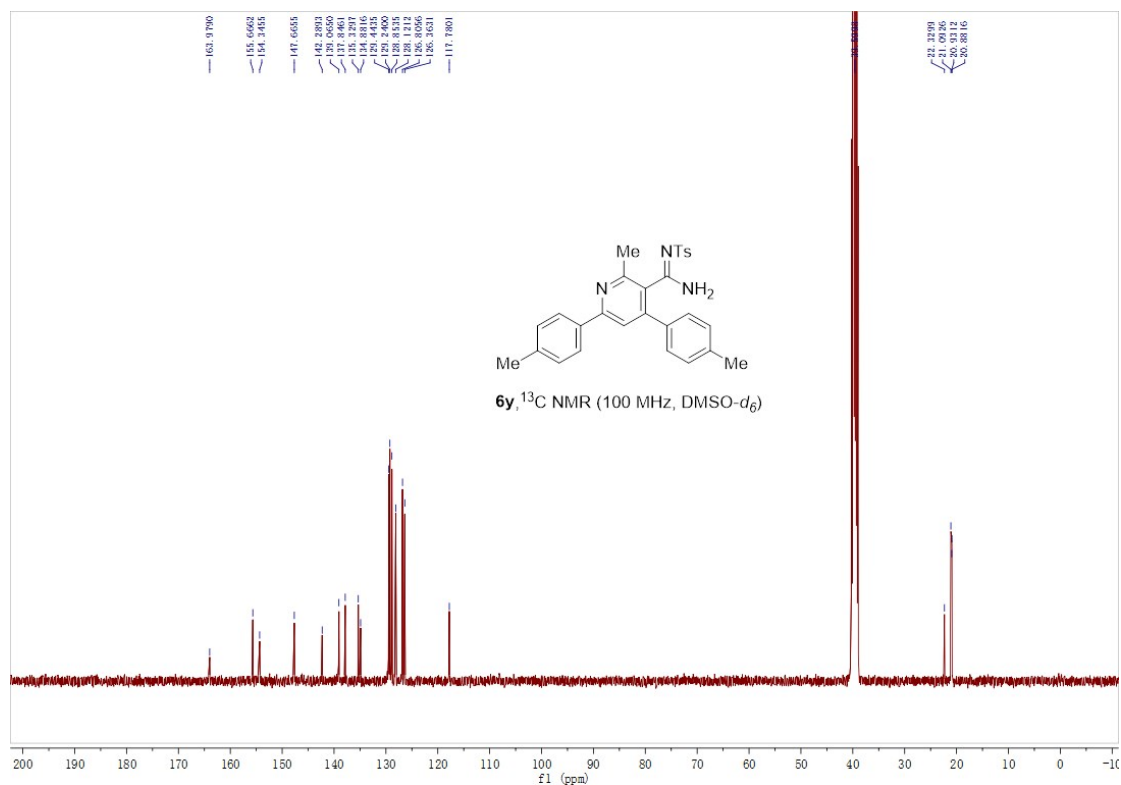
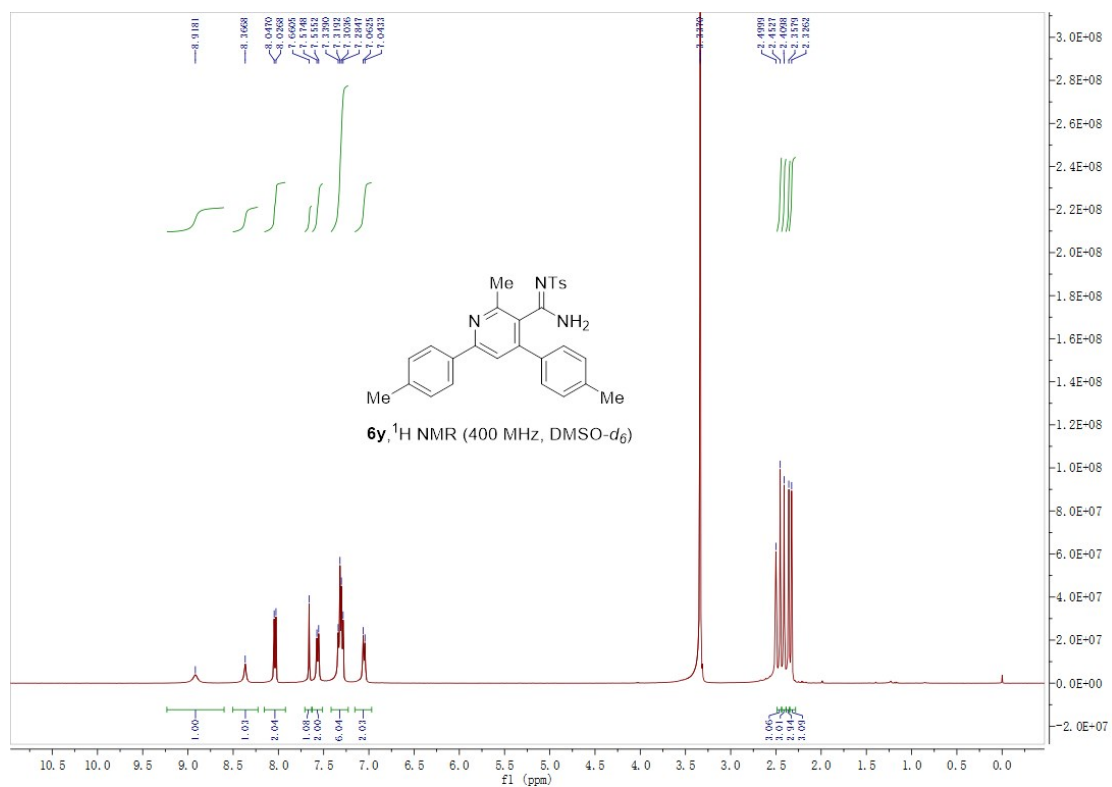


Figure S25. ^1H NMR of **6y** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6y** (100 MHz, $\text{DMSO-}d_6$).

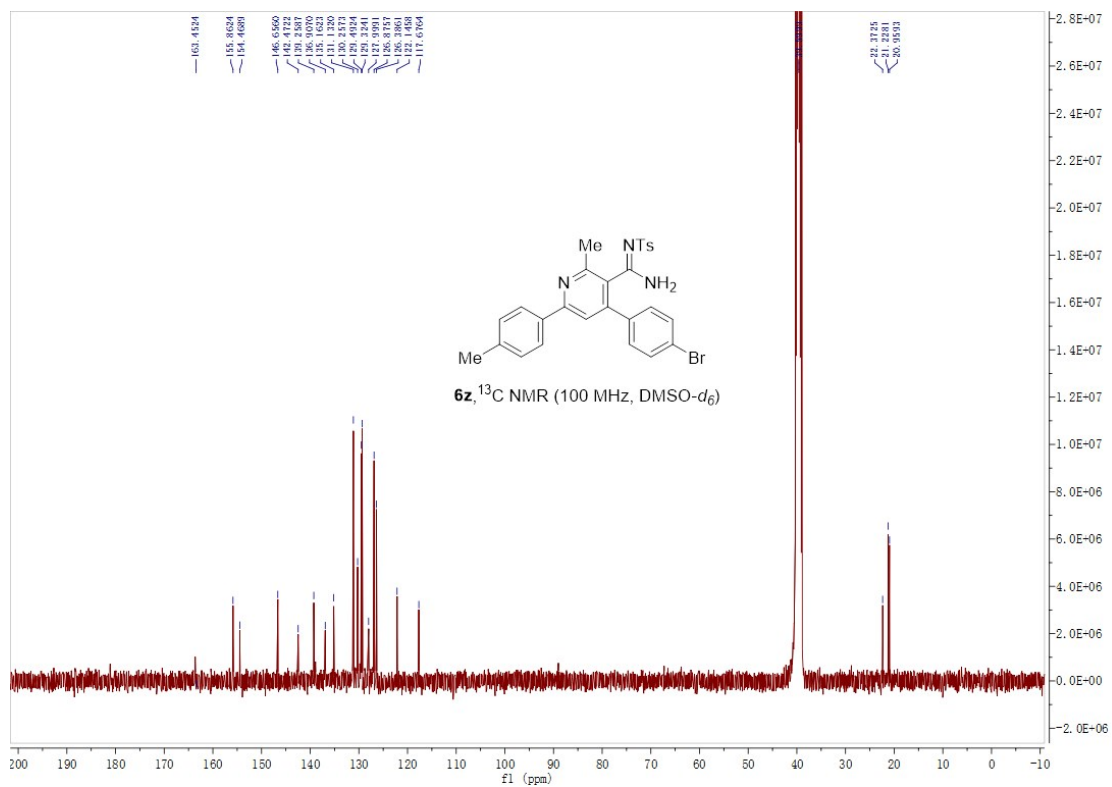
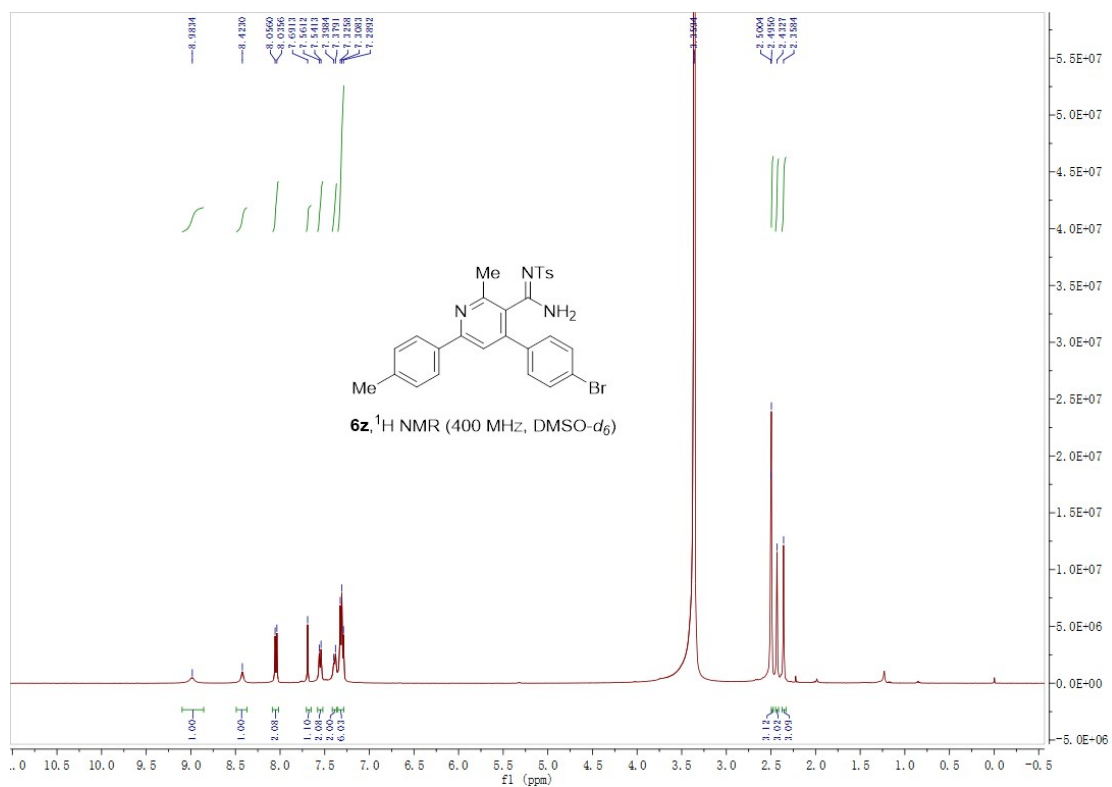


Figure S26. ^1H NMR of **6z** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6z** (100 MHz, $\text{DMSO-}d_6$).

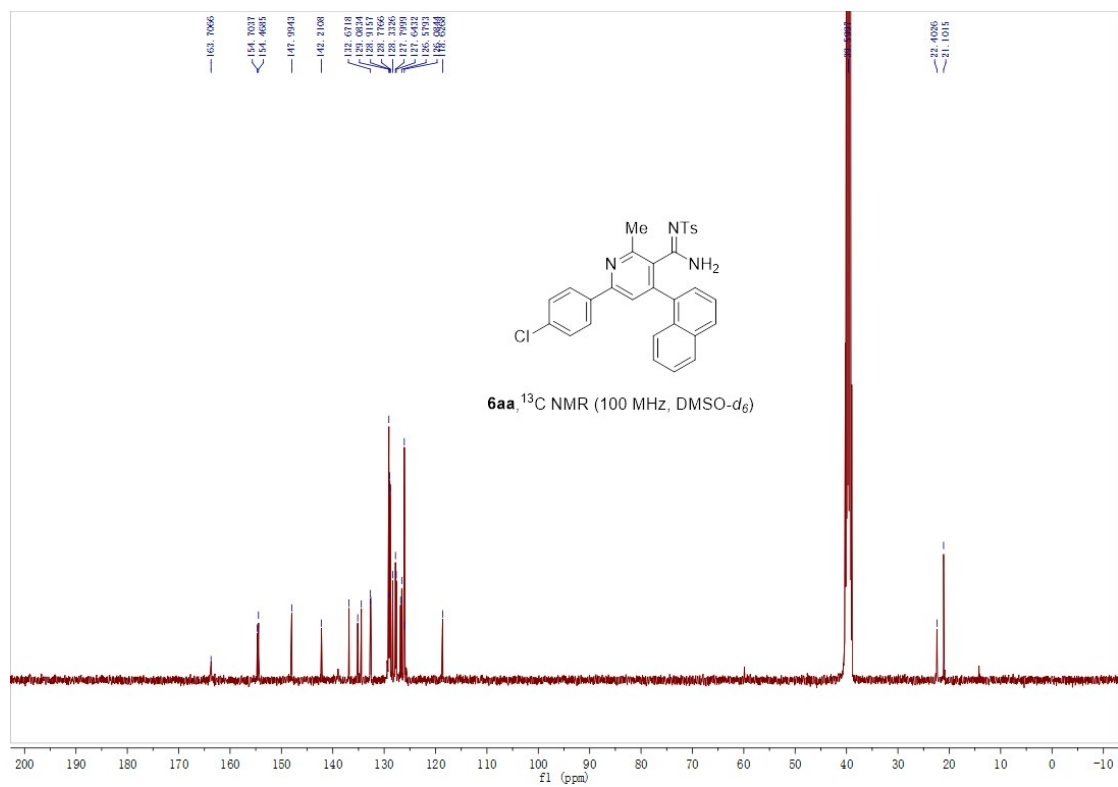
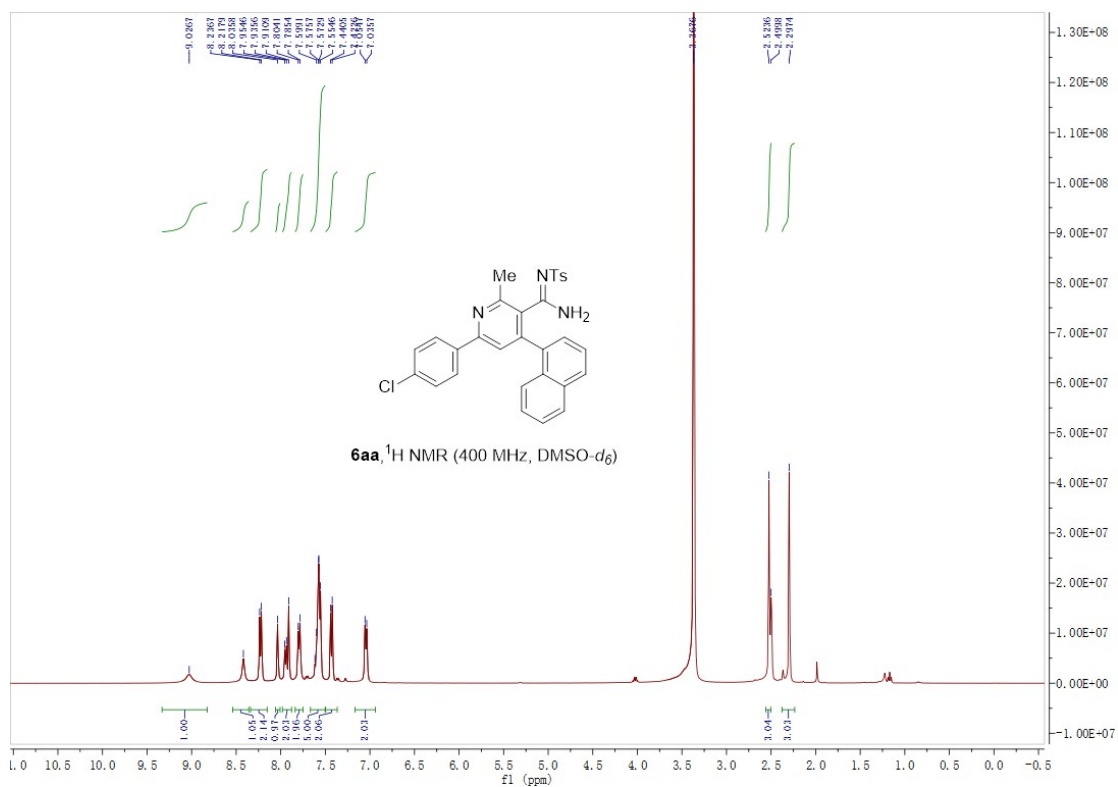


Figure S27. ^1H NMR of **6aa** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **6aa** (100 MHz, $\text{DMSO-}d_6$).

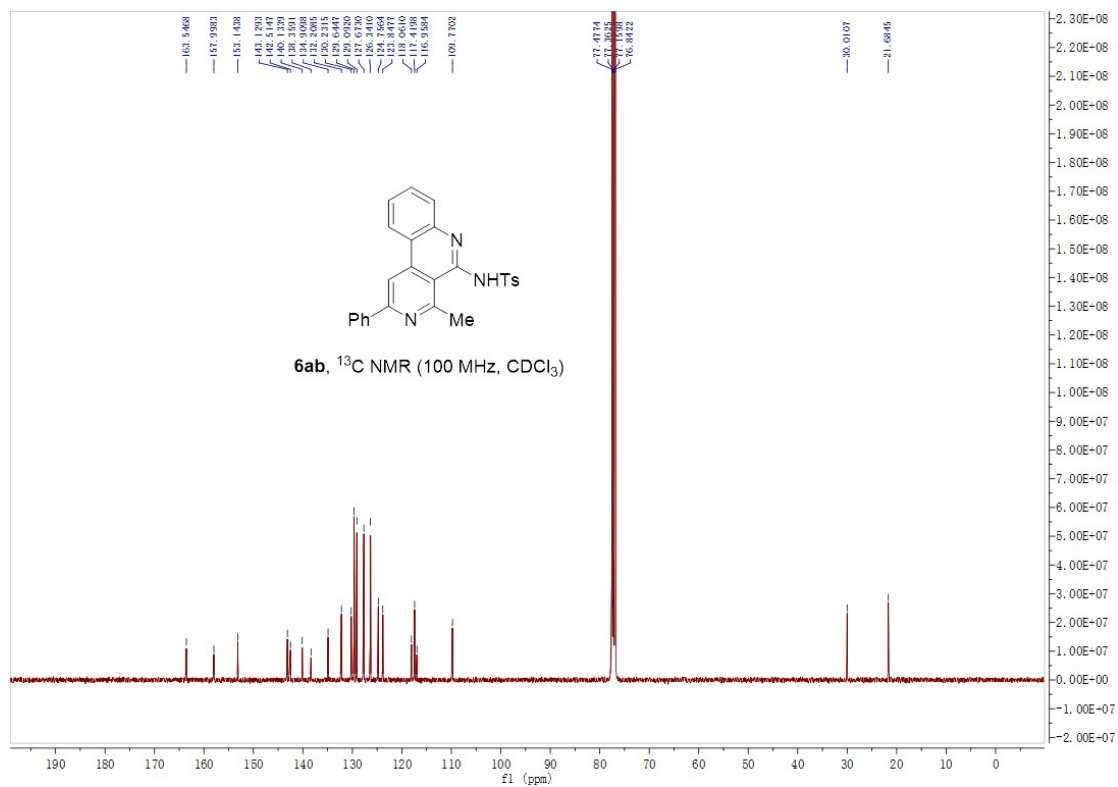
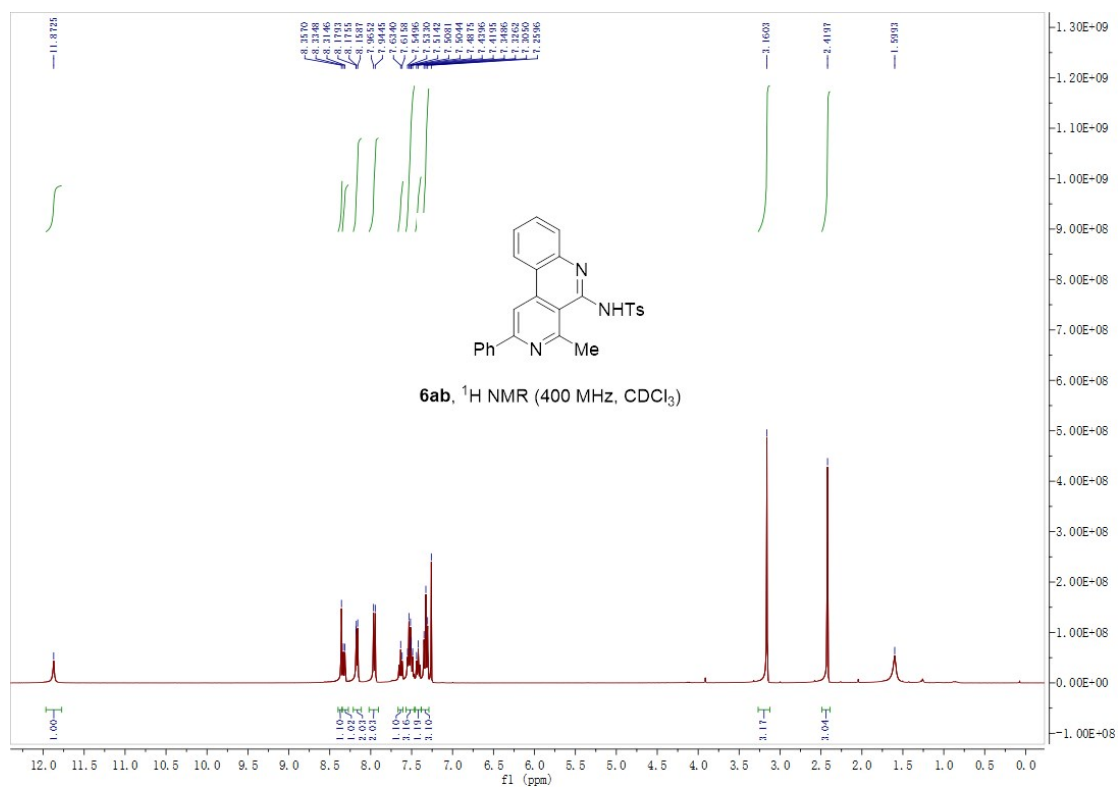


Figure S28. ¹H NMR of **6ab** (400 MHz, CDCl₃) and ¹³C NMR of **6ab** (100 MHz, CDCl₃).

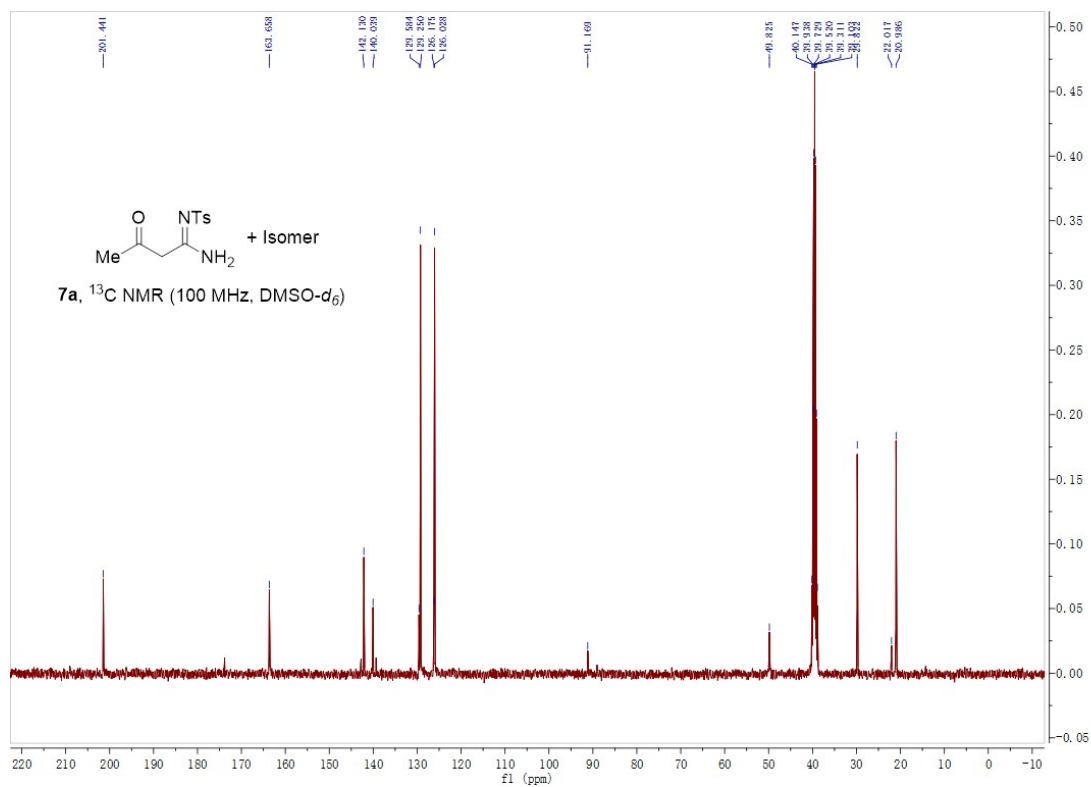
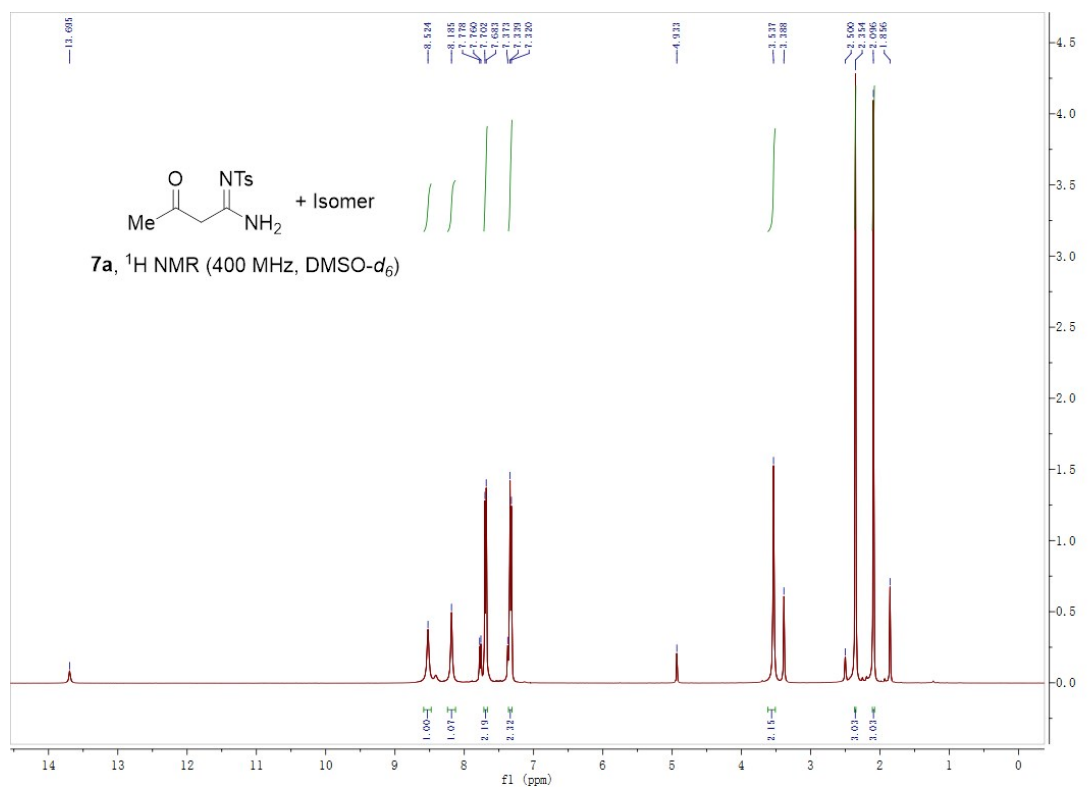
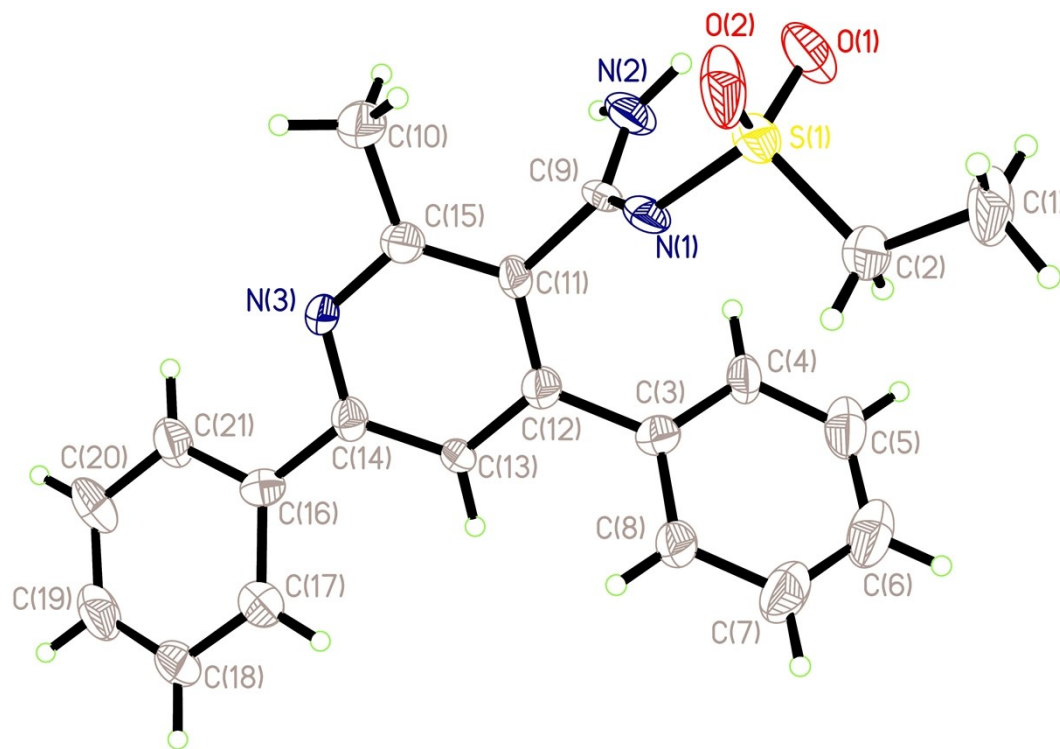


Figure S29. ^1H NMR of **7a** (400 MHz, $\text{DMSO-}d_6$) and ^{13}C NMR of **7a** (100 MHz, $\text{DMSO-}d_6$).

5. X-ray Crystallographic Data for Compound **6j** (CCDC deposition number 2043697)



5. Reference

- [1] Meng, H.; Xu, Z.; Qu, Z.; Huang, H.; Deng, G. J. *Org. Lett.*, **2020**, *22(15)*, 6117-6121.
- [2] Chernyak, D.; Gadamsetty, S. B.; Gevorgyan, V. *Org Lett.*, **2008**, *10(11)*, 2307-2310
- [3] Das, D.; Samanta, R. *Adv. Synth. Catal.*, **2018**, *360*, 379-384.