

Supporting Information

Rhodium(II)-Catalyzed Formal [3+2] Cycloaddition of N-Sulfonyl-1,2,3-Triazoles with Isoxazoles: An Entry to Polysubstituted 3-Aminopyrroles

Xiaoqiang Lei,^{†,‡} Longbo Li,[‡] Yupeng He,^{*,†} and Yefeng Tang^{*,‡,§}

*E-mail: yefengtang@tsinghua.edu.cn
yupeng.he@aliyun.com*

[†]College of Chemistry, Chemical Engineering and Environmental Engineering, Liaoning Shihua University, Dandong Lu West 1, Fushun 113001, China

[‡]Comprehensive AIDS Research Center, Department of Pharmacology & Pharmaceutical Sciences, School of Medicine, Tsinghua University, Beijing 100084, China

[§]Collaborative Innovation Center for Biotherapy, State Key Laboratory of Biotherapy and Cancer Center, West China Hospital, West China Medical School, Sichuan University, Chengdu 610041, China

Table of Contents

1. General Information	S2
2. General Procedures for Preparation of Isoxazoles	S2
3. General Procedures for Transannulation of 1,2,3-Triazoles with Isoxazoles	S3
4. General Procedures for “One-Pot” Synthesis of 3-Aminopyrroles	S3
5. Analysis Data of Isoxazoles	S4
6. Analysis Data of 3-Aminopyrroles	S6
7. NMR Spectra of Isoxazoles	S16
8. NMR Spectra of 3-Aminopyrroles	S22
9. X-ray Crystallographic Structure of 3e	S48

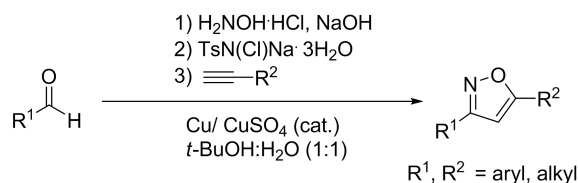
1. General Information

NMR spectra were recorded on Bruker AV400 instrument. TMS was used as internal standard for ^1H NMR (0 ppm), and solvent signal was used as reference for ^{13}C NMR (CDCl_3 , 77.16 ppm; Acetone- d_6 , 29.84 ppm). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, td = triple doublet, qd = quarter doublet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on a Waters Xevo G2 QTOF MS.

Reactions were monitored by Thin Layer Chromatography on plates (GF_{254}) supplied by Yantai Chemicals (China) using UV light as visualizing agent and an ethanolic solution of Potassium permanganate, and heat as developing agents. If not specially mentioned, flash column chromatography uses silica gel (200-300 mesh) supplied by Tsingtao Haiyang Chemicals (China).

Solvent purification was conducted according to Purification of Laboratory Chemicals (Peerrin, D. D.; Armarego, W. L. and Perrins, D. R., Pergamon Press: Oxford, 1980). Yields refer to chromatographically and spectroscopically (^1H NMR) homogeneous materials.

2. General Procedures for Preparation of Isoxazoles¹



Aldehyde (6.0 mmol) was added to a solution of hydroxylamine hydrochloride (0.462 g, 6.6 mmol) in 24 mL of 1:1 $t\text{-BuOH}:\text{H}_2\text{O}$. To this was added NaOH (0.262 g, 6.6 mmol), and after being stirred for 30 min at ambient temperature, TLC analysis indicated that oxime formation was complete. Chloramine-T trihydrate (1.861 g, 6.6 mmol) was added in small portions over 5min, followed by $\text{CuSO}_4\cdot 5\text{H}_2\text{O}$ (0.05 g, 0.18 mmol) and copper turnings (ca. 13 mg). Alkyne (6.6 mmol) was added, pH was adjusted to ca. 6 by addition of a few drops of 1 M NaOH , and stirring was continued for another 6 h. The reaction mixture was poured into ice/water (45.0 mL), and 3.0 mL of dilute NH_4OH was added to remove all copper salts. The product was collected by filtration, redissolved, and passed through a short plug of silica gel affording the corresponding isoxazole.

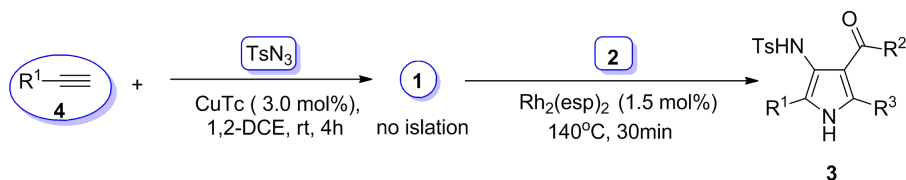
¹Hansen, T. V.; Wu, P.; Fokin, V. V. *J. Org. Chem.* **2005**, *70*, 7761-7764.

3. General Procedures for Transannulation of 1,2,3-Triazoles with Isoxazoles



A 10 mL pressure tube, fitted with a rubber septum, was charged with triazole **1** (0.30 mmol, 1.5 equiv), $\text{Rh}_2(\text{esp})_2$ (2.1 mg, 0.003 mmol, 1.5 mol %) and 3,5-disubstituted isoxazole **2** (0.20 mmol, 1.0 equiv). The reaction vessel was added freshly distilled 1,2-dichloroethane (1.0 mL), sealed with a teflon screwcap and then placed in an oil bath preheated to 140 °C. The resulting solution was heated at this temperature for 0.5 h. After consumption of the triazole monitored by TLC analysis, the reaction was cooled to ambient temperature. The solvent was removed in vacuo, and the resulting residue was submitted to flash chromatography (SiO_2 , hexane/EtOAc) to obtain the corresponding 3-aminopyrrole derivative **3**.

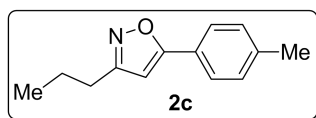
4. General Procedures for Transannulation of N-Sulfonyl-1,2,3-Triazoles with Isoxazoles by “One-Pot”



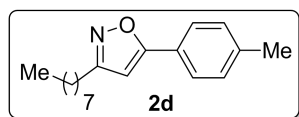
A 10 mL pressure tube, fitted with a rubber septum, was charged with copper(I) thiophene-2-carboxylate (CuTc , 2.9 mg, 0.015 mmol, 0.03 equiv in regards to alkyne), alkyne **4** (0.5 mmol, 1.0 equiv) and 1,2-DCE (1.5 mL). The reaction mixture was cooled in an ice-water bath. Tosyl azide (0.5 mmol, 1.0 equiv) was added slowly, and then the reaction mixture was allowed to warm to room temperature and stir for 4 h. Isoxazole **2** (0.062 g, 0.33 mmol, 0.67 equiv) and $\text{Rh}_2(\text{esp})_2$ (3.815 mg, 0.015 mmol, 1.5 mol %) were added to the above mixture, which was then placed in an oil bath preheated to 140 °C. The resulting solution was kept for stirring at this temperature for 0.5 h. After consumption of the triazole monitored by TLC analysis, the reaction mixture was cooled to ambient temperature. The solvent was removed in vacuo, and the resulting residue was submitted to flash chromatography (SiO_2 , hexane/EtOAc) to obtain the corresponding 3-aminopyrrole.

5. Analysis Data of Isoxazoles

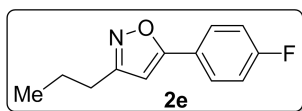
Note: **2k** and **2n** are commercially available compounds and **2a**, **2b**, **2f**, **2h**, **2j**, **2l**, **2o** and **2p** are known compounds.^{1,2} Thus, their ¹H-NMR, ¹³C-NMR and GC-MS datas are not provided. The isoxazoles **2c-2e**, **2g**, **2i** and **2m** are new compounds, and their spectroscopic data are provided below.



3-propyl-5-(p-tolyl)isoxazole (2c): The product was obtained as a colorless solid. (500 mg, 2.49 mmol), Yield: 50%; ¹H NMR (CDCl₃, 400 MHz): δ = 7.65 (d, J = 8.0 Hz, 2H), 7.26-7.24 (m, 2H), 6.32 (s, 1H), 2.68 (t, J = 7.6 Hz, 2H), 2.40 (s, 3H), 1.79-1.70 (m, 2H), 1.02 (t, J = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ = 169.8, 164.6, 140.3, 129.7, 125.8, 125.2, 98.7, 28.2, 21.9, 21.6, 13.9. HRMS m/z calcd for C₁₃H₁₅NO [M+H]⁺: 202.1248; found: 202.1232.



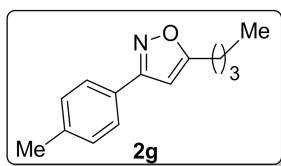
3-octyl-5-(p-tolyl)isoxazole (2d): The product was obtained as a colorless solid. (850 mg, 3.14 mmol), Yield: 52%; ¹H NMR (CDCl₃, 400 MHz): δ = 7.65 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 6.31 (s, 1H), 2.69 (t, J = 7.8 Hz, 2H), 2.39 (s, 3H), 1.73-1.66 (m, 2H), 1.39-1.27 (br, 10H), 0.87 (t, J = 8.0 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ = 169.8, 164.8, 140.3, 129.7, 125.8, 125.2, 98.6, 32.0, 29.4, 29.4, 29.4, 29.3, 28.5, 26.3, 22.8, 21.6, 14.2. HRMS m/z calcd for C₁₈H₂₅NO [M+H]⁺: 272.2025; found: 272.2014.



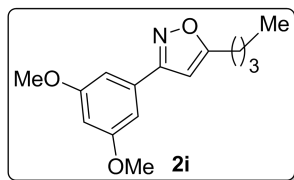
5-(4-fluorophenyl)-3-propylisoxazole (2e): The product was obtained as a colorless solid. (712 mg, 3.47 mmol), Yield: 58%; ¹H NMR (CDCl₃, 400 MHz): δ = 7.76-7.72 (m, 2H), 7.13 (t, J = 8.6 Hz, 2H), 6.32 (s, 1H), 2.68 (t, J = 7.8 Hz, 2H), 1.80-1.69 (m, 2H), 1.01 (t, J = 7.2 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ = 168.6, 164.7, 163.7 (d, J = 249.1 Hz), 127.9 (d, J = 8.4 Hz); 124.2 (d, J = 3.4 Hz), 116.2 (d, J = 21.9 Hz), 99.0 (d, J = 0.8 Hz), 28.1, 21.8, 13.8. HRMS m/z calcd for

²(a) Jawalekar, A. M.; Reubsaet, E.; Rutjes, F. P. J. T.; van Delft, F. L. *Chem. Commun.* **2011**, 47, 3198-3200; (b) Bharate, S. B.; Padala, A. K.; Dar, B. A.; Yadav, R. R.; Singh, B.; Vishwakarm, R, A. *Tetrahedron Lett.* **2013**, 54, 3558-3561. (c) Han, L. Q.; Zhang, B. J.; Zhu, M.; Yan, J. *Tetrahedron Lett.* **2014**, 55, 2308-2311.

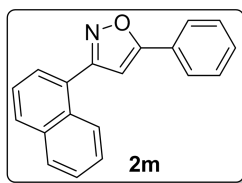
C₁₂H₁₂FNO [M+H]⁺: 206.0983; found: 206.0981.



5-butyl-3-(p-tolyl)isoxazole (2g): The product was obtained as a colorless solid. (680 mg, 3.16 mmol), Yield: 53%; ¹H NMR (CDCl₃, 400 MHz): δ = 7.68 (d, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.25 (s, 1H), 2.77 (t, *J* = 7.6 Hz, 2H), 2.38 (s, 3H), 1.76-1.68 (m, 2H), 1.47-1.38 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ = 174.2, 162.4, 139.9, 129.6, 126.8, 126.8, 98.8, 29.7, 26.6, 22.3, 21.5, 13.8. HRMS *m/z* calcd for C₁₄H₁₇NO [M+H]⁺: 216.1396; found: 216.1388.

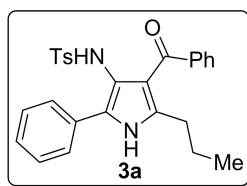


5-butyl-3-(3,5-dimethoxyphenyl)isoxazole (2i): The product was obtained as a yellow solid. (600 mg, 2.68 mmol), Yield: 45%; ¹H NMR (CDCl₃, 400 MHz): δ = 6.94 (d, *J* = 2.0 Hz, 2H), 6.53 (t, *J* = 2.2 Hz, 1H), 6.25 (s, 1H), 3.84 (s, 6H), 2.79 (d, *J* = 7.6 Hz, 2H), 1.77-1.69 (m, 2H), 1.48-1.39 (m, 2H), 0.96 (t, *J* = 7.4 Hz, 3H); ¹³C NMR (CDCl₃, 100 MHz): δ = 174.4, 162.4, 161.2, 131.4, 104.9, 102.3, 99.1, 55.7, 29.7, 26.6, 22.3, 13.8. HRMS *m/z* calcd for C₁₅H₁₉NO₃ [M+H]⁺: 262.1450; found: 262.1443.

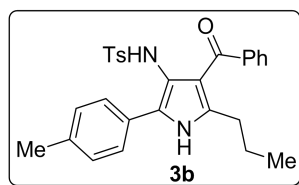


3-(naphthalen-1-yl)-5-phenylisoxazole (2m): The product was obtained as a colorless solid. (908 mg, 3.35 mmol), Yield: 56%; ¹H NMR (CDCl₃, 400 MHz): δ = 8.44-8.42 (m, 1H), 7.96-7.87 (m, 4H), 7.76-7.75 (m, 1H), 7.57-7.46 (m, 6H), 6.83 (s, 1H); ¹³C NMR (CDCl₃, 100 MHz): δ = 169.9, 163.3, 134.0, 131.2, 130.4, 130.4, 129.2, 128.6, 127.9, 127.6, 127.2, 127.1, 126.4, 126.1, 125.8, 125.3, 101.1. HRMS *m/z* calcd for C₁₉H₁₃NO [M+H]⁺: 272.1079; found: 272.1075.

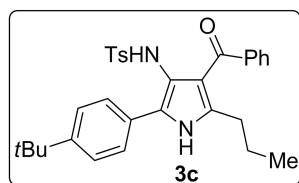
6. Analysis Data of 3-Aminopyrroles



N-(4-benzoyl-2-phenyl-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3a): The product was obtained as a colorless solid. (41.0 mg, 0.089 mmol), Yield: 84%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.22 (s, 1H), 7.77 (d, J = 7.6 Hz, 2H), 7.51-7.47 (m, 2H), 7.42-7.38 (m, 4H), 7.34-7.29 (m, 3H), 7.26-7.24 (m, 2H), 6.88 (d, J = 8.0 Hz, 2H), 2.19 (t, J = 7.6 Hz, 2H), 2.08 (s, 3H), 1.36-1.30 (m, 2H), 0.63 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.9, 143.2, 139.2, 136.7, 135.5, 132.1, 131.0, 129.3, 129.1, 128.8, 128.0, 128.0, 127.8, 127.6, 126.4, 118.5, 117.4, 29.6, 23.2, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{27}\text{H}_{26}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 459.1741; found: 459.1742.

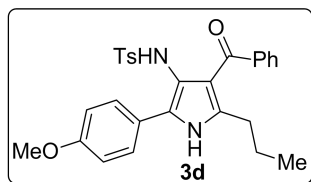


N-(4-benzoyl-5-propyl-2-(p-tolyl)-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3b): The product was obtained as a colorless solid. (55.0 mg, 0.117 mmol), Yield: 73%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.26 (s, 1H), 7.66 (d, J = 8.0 Hz, 2H), 7.51-7.46 (m, 2H), 7.40 (d, J = 8.4 Hz, 2H), 7.33-7.30 (m, 2H), 7.23 (d, J = 6.8 Hz, 2H), 7.19 (d, J = 8.0 Hz, 2H), 6.88 (d, J = 8.0 Hz, 2H), 2.36 (s, 3H), 2.16 (t, J = 7.6 Hz, 2H), 2.08 (s, 3H), 1.36-1.27 (m, 2H), 0.61 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 193.0, 143.2, 139.2, 137.4, 136.6, 135.4, 132.0, 129.5, 129.2, 129.0, 128.1, 128.0, 127.9, 126.3, 118.2, 116.9, 29.5, 23.2, 21.5, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 473.1902; found: 473.1899.



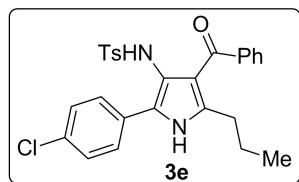
N-(4-benzoyl-2-(4-(tert-butyl)phenyl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3c): The product was obtained as a colorless solid. (77.0 mg, 0.15 mmol), Yield: 80%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.20 (s, 1H), 7.71 (d, J = 8.4 Hz, 2H), 7.50-7.47 (m, 2H), 7.43-7.41 (m,

4H), 7.32 (t, $J = 7.6$ Hz, 2H), 7.26-7.24 (m, 1H), 6.88 (d, $J = 8.0$ Hz, 2H), 2.19 (t, $J = 7.6$ Hz, 2H), 2.07 (s, 3H), 1.34-1.26 (s and m, 12H), 0.62 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): $\delta = 192.9, 150.6, 143.2, 139.2, 136.4, 135.5, 132.1, 129.2, 129.1, 128.1, 128.0, 128.0, 128.0, 126.0, 125.7, 118.5, 116.9, 34.8, 31.4, 29.6, 23.2, 21.4, 13.6$; HRMS m/z calcd for $\text{C}_{31}\text{H}_{34}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 515.2358; found: 515.2368.



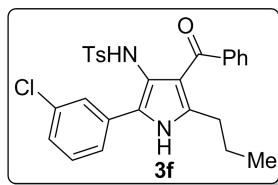
N-(4-benzoyl-2-(4-methoxyphenyl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide

(3d): The product was obtained as a colorless solid. (50.0 mg, 0.103 mmol), Yield: 61%; ^1H NMR (CDCl_3 , 400 MHz): $\delta = 8.03$ (s, 1H), 7.32 (t, $J = 7.8$ Hz, 2H), 7.50-7.41 (m, 4H), 7.32 (t, $J = 7.8$ Hz, 2H), 7.26-7.23 (m, 2H), 6.96 (d, $J = 8.8$ Hz, 2H), 6.89 (d, $J = 8.0$ Hz, 2H), 3.85 (s, 3H), 2.18 (t, $J = 7.6$ Hz, 2H), 2.09 (s, 3H), 1.37-1.31 (m, 2H), 0.64 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): $\delta = 192.9, 159.2, 143.2, 139.1, 136.1, 135.5, 132.1, 129.2, 129.1, 128.0, 128.0, 127.9, 127.8, 123.5, 118.3, 116.5, 114.3, 55.4, 29.6, 23.2, 21.4, 13.6$; HRMS m/z calcd for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$: 489.185; found: 489.1848.



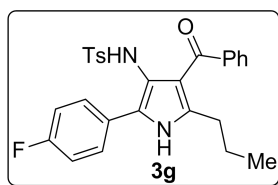
N-(4-benzoyl-2-(4-chlorophenyl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3e):

The product was obtained as a colorless solid. (51.0 mg, 0.107 mmol), Yield: 60%; ^1H NMR (CDCl_3 , 400 MHz): $\delta = 8.15$ (s, 1H), 7.70 (d, $J = 8.4$ Hz, 2H), 7.51-7.48 (m, 2H), 7.40 (d, $J = 8.0$ Hz, 2H), 7.37-7.31 (m, 4H), 7.26-7.24 (m, 2H), 6.89 (d, $J = 8.0$ Hz, 2H), 2.20 (t, $J = 7.6$ Hz, 2H), 2.09 (s, 3H), 1.37-1.31 (m, 2H), 0.64 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): $\delta = 192.9, 143.4, 138.9, 136.9, 135.3, 133.4, 132.2, 129.4, 129.3, 129.0, 129.0, 128.0, 128.0, 127.6, 126.6, 118.5, 117.9, 29.6, 23.2, 21.4, 13.6$; HRMS m/z calcd for $\text{C}_{27}\text{H}_{25}\text{ClN}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 493.1351; found: 493.1353.



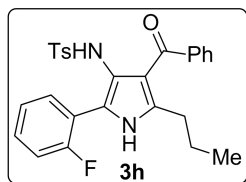
N-(4-benzoyl-2-(3-chlorophenyl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3f):

The product was obtained as a colorless solid. (46.0 mg, 0.095 mmol), Yield: 50%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.24 (s, 1H), 7.76 (d, J = 7.6 Hz, 1H), 7.61 (s, 1H), 7.52-7.48 (m, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.35-7.29 (m, 3H), 7.26-7.22 (m, 3H), 6.90 (d, J = 8.0 Hz, 2H), 2.20-2.18 (m, 2H), 2.10 (s, 3H), 1.37-1.31 (m, 2H), 0.63 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.9, 143.4, 139.0, 137.2, 135.3, 134.5, 132.7, 132.2, 130.1, 129.3, 129.0, 128.0, 127.9, 127.5, 126.3, 126.0, 125.0, 118.6, 118.2, 29.6, 23.2, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{27}\text{H}_{25}\text{ClN}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 493.1349; found: 493.1353.



N-(4-benzoyl-2-(4-fluorophenyl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3g):

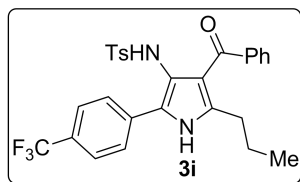
The product was obtained as a colorless solid. (53.0 mg, 0.111 mmol), Yield: 61%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.27 (s, 1H), 7.75-7.72 (m, 2H), 7.52-7.48 (m, 2H), 7.40 (d, J = 8.0 Hz, 2H), 7.33 (t, J = 7.6 Hz, 2H), 7.26-7.23 (m, 2H), 7.09-7.05 (m, 2H), 6.89 (d, J = 8.0 Hz, 2H), 2.18 (t, J = 7.6 Hz, 2H), 2.09 (s, 3H), 1.35-1.30 (m, 2H), 0.62 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 193.0, 162.2 (d, J = 246.0 Hz), 143.4, 139.0, 136.8, 135.3, 132.2, 129.3, 129.0, 128.4, 128.3, 128.0, 128.0, 127.2, 127.2, 127.0, 118.3, 117.3, 115.8 (d, J = 25.2 Hz), 29.5, 23.3, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{27}\text{H}_{25}\text{FN}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 477.1647; found: 477.1648.



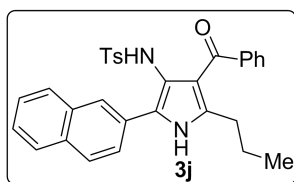
N-(4-benzoyl-2-(2-fluorophenyl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3h):

The product was obtained as a colorless solid. (49.0 mg, 0.103 mmol), Yield: 51%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.60 (s, 1H), 8.33-8.29 (m, 1H), 7.66 (s, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.43 (d, J = 8.0 Hz, 2H), 7.33 (t, J = 7.8 Hz, 2H), 7.26-7.21 (m, 4H), 7.15-7.10 (m, 1H), 6.91 (d, J

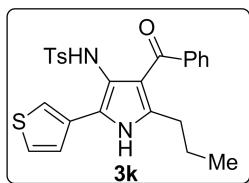
= 8.0 Hz, 2H), 2.19 (t, J = 7.6 Hz, 2H), 2.10 (s, 3H), 1.39-1.29 (m, 2H), 0.65 (t, J = 7.8 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 193.1, 159.1 (d, J = 242.4 Hz), 143.3, 139.1, 136.6, 135.2, 132.1, 130.2, 130.2, 129.3, 129.1, 129.0, 129.0, 128.0, 128.0, 124.7, 124.7, 121.9, 119.3, 118.4 (d, J = 11.2 Hz), 117.7, 115.9, 116.0, 115.7, 29.6, 23.0, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{27}\text{H}_{25}\text{FN}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 477.1650; found: 477.1648.



N-(4-benzoyl-5-propyl-2-(4-(trifluoromethyl)phenyl)-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3i): The product was obtained as a colorless solid. (47.0 mg, 0.089 mmol), Yield: 40 %; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.37 (s, 1H), 7.88 (d, J = 8.0 Hz, 2H), 7.61 (m, 3H), 7.51 (t, J = 7.4 Hz, 1H), 7.39 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.26-7.24 (m, 2H), 6.88 (d, J = 8.0 Hz, 2H), 2.21 (t, J = 7.6 Hz, 2H), 2.08 (s, 3H), 1.37-1.29 (m, 2H), 0.63 (t, J = 7.4 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 193.1, 144.0, 140.3, 139.1, 138.9, 136.9, 136.0, 132.6, 130.0, 129.8, 128.9, 128.4 (q, J = 31.9 Hz), 128.3, 127.6, 125.8 (q, J = 3.8 Hz), 125.5 (q, J = 269.4 Hz), 119.9, 119.8, 119.2, 24.1, 21.3, 13.7; HRMS m/z calcd for $\text{C}_{28}\text{H}_{25}\text{F}_3\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 527.1617; found: 527.1616.

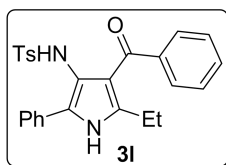


N-(4-benzoyl-2-(naphthalen-2-yl)-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3j): The product was obtained as a colorless solid. (56.0 mg, 0.110 mmol), Yield: 61%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.24 (s, 1H), 8.06 (d, J = 8.0 Hz, 1H), 8.00 (s, 1H), 7.87-7.82 (m, 3H), 7.57 (s, 1H), 7.52-7.46 (m, 3H), 7.41 (d, J = 8.0 Hz, 2H), 7.35 (t, J = 7.2 Hz, 2H), 7.30-7.28 (m, 2H), 6.84 (d, J = 8.0 Hz, 2H), 2.24 (t, J = 7.6 Hz, 2H), 2.04 (s, 3H), 1.41-1.36 (m, 2H), 0.67 (t, J = 7.2 Hz, 3H); ^{13}C NMR ($(\text{CD}_3)_2\text{SO}$, 100 MHz): δ = 191.8, 142.1, 139.6, 137.0, 136.9, 132.9, 131.8, 131.7, 129.2, 128.7, 128.4, 128.1, 127.8, 127.7, 127.5, 127.3, 126.5, 126.3, 125.8, 125.2, 124.8, 120.1, 115.0, 28.4, 23.3, 20.7, 13.5; HRMS m/z calcd for $\text{C}_{31}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 509.1900; found: 509.1899.

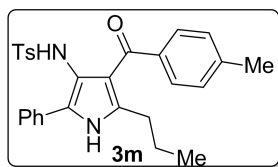


N-(4-benzoyl-5-propyl-2-(thiophen-3-yl)-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3k):

The product was obtained as a colorless solid. (56.0 mg, 0.121 mmol), Yield: 63%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.26 (s, 1H), 7.65-7.64 (m, 2H), 7.51-7.49 (m, 1H), 7.45 (d, J = 8.0 Hz, 3H), 7.41 (s, 1H), 7.36-7.30 (m, 3H), 7.26-7.24 (m, 2H), 6.89 (d, J = 7.6 Hz, 2H), 2.19 (t, J = 7.6 Hz, 2H), 2.06 (s, 3H), 1.37-1.31 (m, 2H), 0.63 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.7, 143.4, 139.0, 136.2, 135.4, 132.2, 131.1, 129.3, 129.1, 128.1, 128.0, 126.2, 125.9, 125.1, 120.7, 118.2, 116.7, 29.6, 23.3, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{25}\text{H}_{24}\text{N}_2\text{O}_3\text{S}_2$ $[\text{M}+\text{H}]^+$: 465.1302; found: 465.1307.



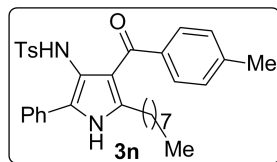
N-(4-benzoyl-5-methyl-2-phenyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3l): The product was obtained as a colorless solid. (69.0 mg, 0.155 mmol), Yield: 73%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.14 (s, 1H), 7.78 (d, J = 8.4 Hz, 2H), 7.51-7.48 (m, 2H), 7.43-7.40 (m, 4H), 7.35-7.30 (m, 3H), 7.27-7.26 (m, 2H), 6.88 (d, J = 8.0 Hz, 2H), 2.07 (s, 3H), 0.98 (t, J = 7.4 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.8, 143.2, 139.1, 137.6, 135.5, 132.2, 130.9, 129.3, 129.1, 128.8, 128.0, 128.0, 127.9, 127.7, 126.4, 118.0, 117.5, 21.4, 21.0, 13.7. HRMS m/z calcd for $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 445.1585; found: 445.1586.



4-methyl-N-(4-(4-methylbenzoyl)-2-phenyl-5-propyl-1H-pyrrol-3-yl)benzenesulfonamide

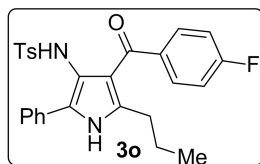
(3m): The product was obtained as a colorless solid. (83.0 mg, 0.176 mmol), Yield: 87%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.29 (s, 1H), 7.76 (d, J = 7.2 Hz, 2H), 7.48 (s, 1H), 7.38 (t, J = 8.6 Hz, 4H), 7.27 (t, J = 7.4 Hz, 1H), 7.17 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 6.85 (d, J = 8.0 Hz, 2H), 2.41 (s, 3H), 2.23 (t, J = 7.6 Hz, 2H), 2.06 (s, 3H), 1.38-1.29 (m, 2H), 0.64 (t, J = 7.4

Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.6, 143.1, 142.8, 136.3, 136.2, 135.4, 131.0, 129.4, 129.2, 128.7, 128.6, 128.0, 127.7, 127.5, 126.4, 118.6, 117.2, 29.5, 23.2, 21.8, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 473.1897; found: 473.1899.



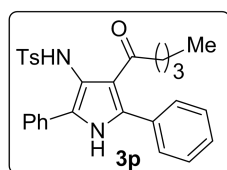
N-(5-ethyl-4-(4-methylbenzoyl)-2-phenyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3n):

The product was obtained as a colorless solid. (68.0 mg, 0.126 mmol), Yield: 63%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.14 (s, 1H), 7.78 (d, J = 7.2 Hz, 2H), 7.47 (s, 1H), 7.41-7.39 (m, 4H), 7.29 (d, J = 7.6 Hz, 1H), 7.17 (d, J = 8.0 Hz, 2H), 7.11 (d, J = 8.0 Hz, 2H), 6.86 (d, J = 8.0 Hz, 2H), 2.41 (s, 3H), 2.25 (t, J = 7.6 Hz, 2H), 2.06 (s, 3H), 1.32-1.29 (m, 2H), 1.22-1.19 (m, 2H), 1.12 (br. 4H), 1.00 (br, 4H), 0.84 (t, J = 7.0 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.5, 143.1, 142.8, 136.4, 136.4, 135.5, 131.0, 129.4, 129.2, 128.8, 128.6, 128.0, 127.7, 127.6, 126.4, 118.5, 117.4, 31.9, 29.9, 29.1, 29.1, 29.1, 27.7, 22.7, 21.7, 21.4, 14.2; HRMS m/z calcd for $\text{C}_{33}\text{H}_{38}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 543.2683; found: 543.2681.

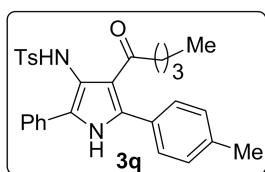


N-(4-(4-fluorobenzoyl)-2-phenyl-5-propyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3o):

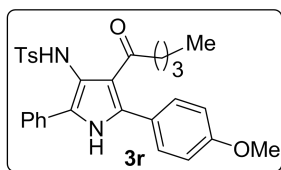
The product was obtained as a colorless solid. (59.0 mg, 0.124 mmol), Yield: 62%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.20 (s, 1H), 7.74 (d, J = 7.6 Hz, 2H), 7.41-7.38 (m, 5H), 7.34-7.29 (m, 3H), 7.01 (t, J = 8.6 Hz, 2H), 6.67 (d, J = 8.0 Hz, 2H), 2.23 (t, J = 7.6 Hz, 2H), 2.10 (s, 3H), 1.39-1.33 (m, 2H), 0.67 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 191.2, 165.3 (d, J = 252.3 Hz), 143.2, 136.1, 136.1, 135.5, 135.3, 131.8, 131.7, 130.8, 129.2, 128.8, 128.0, 127.7, 126.4, 118.5, 117.2, 115.1 (d, J = 21.7 Hz), 29.7, 23.2, 21.4, 13.6; HRMS m/z calcd for $\text{C}_{27}\text{H}_{25}\text{FN}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 477.1649; found: 477.1648.



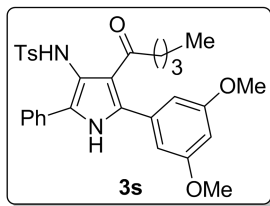
N-(2,5-diphenyl-4-propionyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3p): The product was obtained as a colorless solid. (48.0 mg, 0.102 mmol), Yield: 57%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.20 (s, 1H), 7.94 (s, 1H), 7.75 (d, J = 7.2 Hz, 2H), 7.49-7.28 (m, 10H), 7.10 (d, J = 8.4 Hz, 2H), 2.32 (s, 3H), 1.82 (t, J = 7.6 Hz, 2H), 1.12-1.06 (m, 2H), 0.97-0.88 (m, 2H), 0.67 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 199.9, 143.2, 136.1, 135.1, 132.3, 131.0, 129.4, 129.3, 129.1, 129.0, 128.8, 128.1, 128.1, 127.8, 126.5, 119.1, 118.4, 41.0, 26.2, 22.3, 21.6, 13.8; HRMS m/z calcd for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 473.1906; found: 473.1899.



4-methyl-N-(2-phenyl-4-propionyl-5-(p-tolyl)-1H-pyrrol-3-yl)benzenesulfonamide (3q): The product was obtained as a colorless solid. (52.0 mg, 0.107 mmol), Yield: 55%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.21 (s, 1H), 7.94 (s, 1H), 7.73 (d, J = 7.6 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.37 (t, J = 7.4 Hz, 2H), 7.28-7.20 (m, 5H), 7.09 (d, J = 8.0 Hz, 2H), 2.40 (s, 3H), 2.31 (s, 3H), 1.83 (t, J = 7.4 Hz, 2H), 1.11-1.06 (m, 2H), 0.98-0.90 (m, 2H), 0.68 (t, J = 7.2 Hz, 3H); ^{13}C NMR ($(\text{CD}_3)_2\text{CO}$, 100 MHz): δ = 199.7, 143.9, 139.5, 137.3, 136.2, 132.3, 130.5, 130.3, 129.8, 129.8, 128.9, 128.8, 128.6, 127.8, 127.7, 120.1, 118.5, 41.6, 26.8, 22.9, 21.4, 21.3, 14.1; HRMS m/z calcd for $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 487.2048; found: 487.2055.

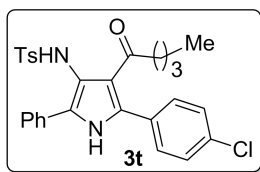


N-(5-(4-methoxyphenyl)-2-phenyl-4-propionyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3r): The product was obtained as a colorless solid. (72.0 mg, 0.144 mmol), Yield: 72%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.23 (s, 1H), 7.96 (s, 1H), 7.73 (d, J = 8.0 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.36 (t, J = 7.6 Hz, 2H), 7.28-7.23 (m, 3H), 7.09 (d, J = 8.4 Hz, 2H), 6.95 (d, J = 8.4 Hz, 2H), 3.85 (s, 3H), 3.32 (s, 3H), 1.83 (t, J = 7.6 Hz, 2H), 1.11-1.05 (m, 2H), 0.97-0.91 (m, 2H), 0.69 (t, J = 7.4 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 199.9, 160.5, 143.2, 136.1, 135.2, 131.0, 130.6, 129.1, 128.8, 128.1, 127.7, 127.7, 126.5, 124.4, 118.7, 118.2, 114.4, 55.6, 40.8, 26.3, 22.4, 21.6, 13.9; HRMS m/z calcd for $\text{C}_{29}\text{H}_{30}\text{N}_2\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$: 503.1999; found: 503.2005.



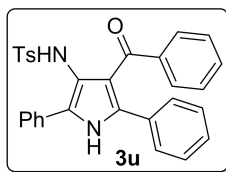
N-(5-(3,5-dimethoxyphenyl)-2-phenyl-4-propionyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3s):

The product was obtained as a colorless solid. (50.0 mg, 0.094 mmol), Yield: 47%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.23 (s, 1H), 7.91 (s, 1H), 7.74 (d, J = 7.2 Hz, 2H), 7.47 (d, J = 8.0 Hz, 2H), 7.38 (t, J = 8.0 Hz, 2H), 7.30-7.28 (m, 1H), 7.10 (d, J = 8.0 Hz, 2H), 6.51 (t, J = 2.0 Hz, 1H), 6.45 (d, J = 2.0 Hz, 2H), 3.80 (s, 6H), 2.32 (s, 3H), 1.91 (t, J = 7.6 Hz, 2H), 1.18-1.11 (m, 2H), 1.03-0.94 (m, 2H), 0.71 (t, J = 7.2 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 200.0, 161.1, 143.2, 136.1, 134.9, 134.0, 130.9, 129.2, 128.8, 128.1, 128.0, 127.8, 126.5, 119.0, 118.2, 107.5, 101.1, 55.7, 40.9, 26.3, 22.4, 21.6, 13.9; HRMS m/z calcd for $\text{C}_{30}\text{H}_{32}\text{N}_2\text{O}_5\text{S}$ $[\text{M}+\text{H}]^+$: 533.2102; found: 533.2110.



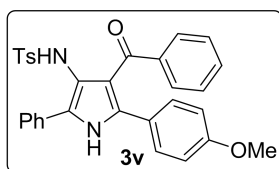
N-(5-(4-chlorophenyl)-2-phenyl-4-propionyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3t):

The product was obtained as a colorless solid. (32.0 mg, 0.064 mmol), Yield: 35%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.22 (s, 1H), 7.86 (s, 1H), 7.72 (d, J = 7.6 Hz, 2H), 7.47-7.42 (m, 4H), 7.38 (t, J = 7.6 Hz, 2H), 7.31-7.27 (m, 3H), 7.10 (d, J = 8.0 Hz, 2H), 7.32 (s, 3H), 1.84 (t, J = 7.6 Hz, 2H), 1.17-1.10 (m, 2H), 1.02-0.93 (m, 2H), 0.71 (t, J = 7.4 Hz, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 199.7, 143.3, 136.0, 135.6, 133.5, 130.8, 130.6, 130.5, 129.2, 129.1, 128.8, 128.6, 128.0, 127.9, 126.6, 119.5, 118.3, 41.1, 26.2, 22.3, 21.6, 13.9; HRMS m/z calcd for $\text{C}_{28}\text{H}_{27}\text{ClN}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 507.1511; found: 507.1509.



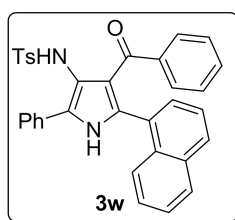
N-(4-benzoyl-2,5-diphenyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3u): The product was obtained as a colorless solid. (40.0 mg, 0.082 mmol), Yield: 41%; ^1H NMR (CDCl_3 , 400

MHz): δ = 8.39 (s, 1H), 7.89 (d, J = 7.6 Hz, 2H), 7.65 (s, 1H), 7.46-7.41 (m, 4H), 7.32 (t, J = 7.4 Hz, 1H), 7.20 (t, J = 7.2 Hz, 1H), 7.14 (d, J = 7.2 Hz, 2H), 7.07-7.01 (m, 5H), 6.96 (t, J = 7.6 Hz, 2H), 6.76 (d, J = 8.0 Hz, 2H), 1.89 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.4, 143.2, 137.0, 135.3, 135.2, 132.0, 131.2, 130.1, 130.0, 129.7, 129.3, 128.9, 128.5, 128.4, 128.2, 128.0, 127.9, 127.2, 126.6, 119.0, 118.1, 21.3; HRMS m/z calcd for $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 493.1584; found: 493.1586.



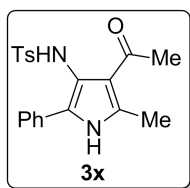
N-(4-benzoyl-5-(4-methoxyphenyl)-2-phenyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide

(3v): The product was obtained as a colorless solid. (68.0 mg, 0.131 mmol), Yield: 65%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.31 (s, 1H), 7.88 (d, J = 7.6 Hz, 2H), 7.65 (s, 1H), 7.33-7.30 (m, 4H), 7.31 (t, J = 7.2 Hz, 1H), 7.22 (t, J = 7.4 Hz, 1H), 7.14 (d, J = 7.6 Hz, 2H), 7.00 - 6.93 (m, 4H), 6.76 (d, J = 7.6 Hz, 2H), 6.58 (d, J = 8.4 Hz, 2H), 3.68 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 192.5, 159.6, 143.2, 137.1, 135.5, 135.2, 131.9, 130.9, 130.0, 129.7, 129.3, 129.2, 128.9, 127.9, 127.9, 127.3, 126.5, 123.7, 118.9, 117.6, 114.0, 55.4, 21.3; HRMS m/z calcd for $\text{C}_{31}\text{H}_{26}\text{N}_2\text{O}_4\text{S}$ $[\text{M}+\text{H}]^+$: 523.1686; found: 523.1692.

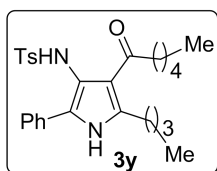


N-(4-benzoyl-5-(naphthalen-1-yl)-2-phenyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide

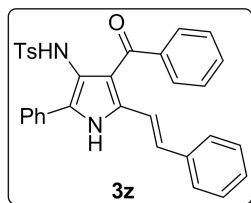
(3w): The product was obtained as a colorless solid. (66.0 mg, 0.122 mmol), Yield: 60%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.47 (s, 1H), 7.94 (d, J = 7.6 Hz, 2H), 7.88 (s, 1H), 7.77 (d, J = 8.4 Hz, 1H), 7.70 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.52-7.42 (m, 6H), 7.34 (t, J = 7.4 Hz, 1H), 7.17-7.09 (m, 2H), 6.92-6.82 (m, 5H), 6.58 (t, J = 7.6 Hz, 2H), 1.92 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 193.1, 143.3, 137.4, 135.1, 134.1, 133.3, 131.9, 131.3, 130.7, 129.4, 129.2, 129.1, 129.0, 128.9, 128.7, 128.7, 128.4, 127.9, 127.9, 126.9, 126.6, 126.4, 126.1, 124.8, 124.7, 119.8, 118.7, 21.2; HRMS m/z calcd for $\text{C}_{34}\text{H}_{26}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 543.1742; found: 543.1742.



N-(4-acetyl-5-methyl-2-phenyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3x): The product was obtained as a colorless solid. (38.0 mg, 0.103 mmol), Yield: 51%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.77 (s, 1H), 7.87 (s, 1H), 7.55 (d, J = 7.6 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.24-7.13 (m, 3H), 7.04 (d, J = 8.0 Hz, 2H), 2.35 (s, 3H), 2.33 (s, 3H), 2.02 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ = 195.6, 143.3, 135.6, 133.0, 130.9, 128.9, 128.5, 128.0, 127.2, 126.4, 126.3, 118.2, 117.4, 29.7, 21.6, 15.0; HRMS m/z calcd for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 369.1273; found: 369.1273.



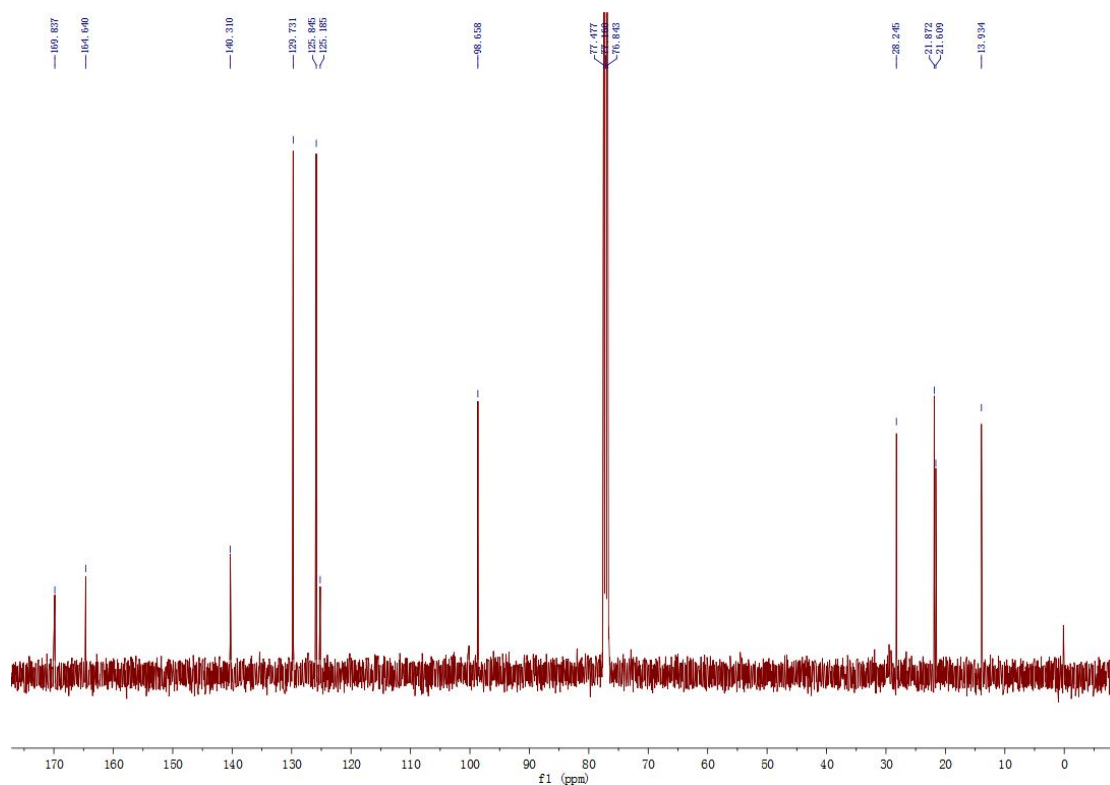
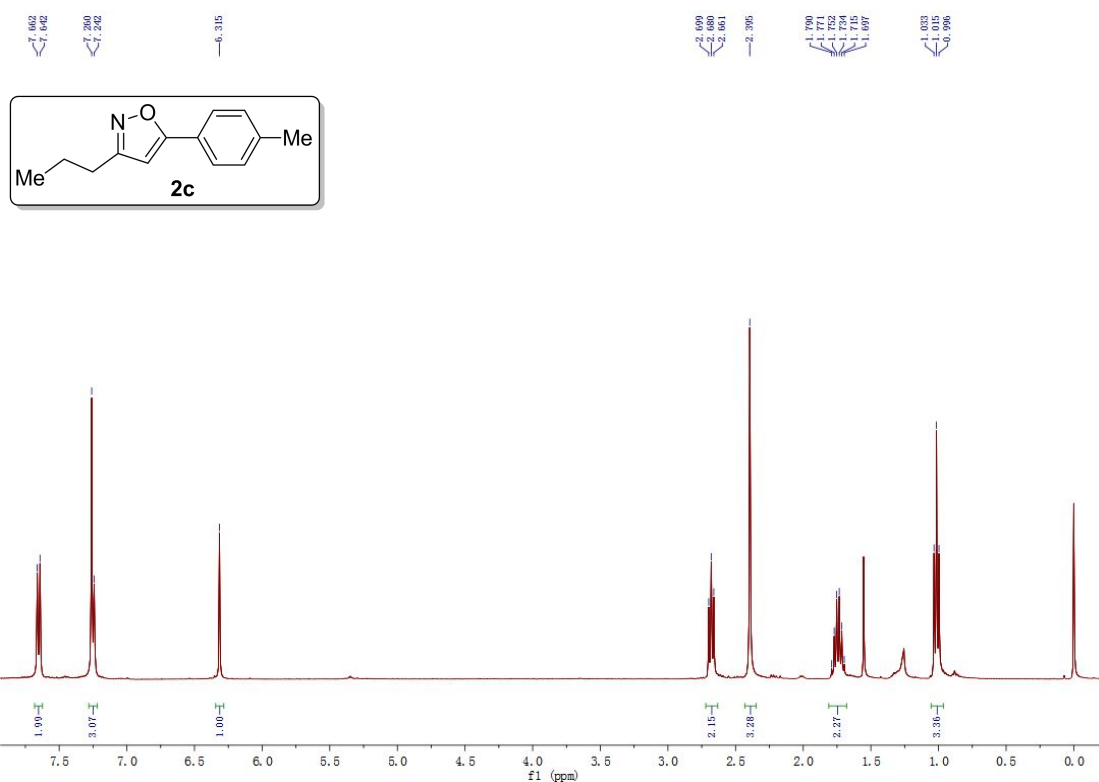
N-(5-ethyl-2-phenyl-4-propionyl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3y): The product was obtained as a colorless solid. (68.0 mg, 0.146 mmol), Yield: 81%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.14 (s, 1H), 7.95 (s, 1H), 7.61 (d, J = 7.6 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.24-7.22 (m, 1H), 7.05 (d, J = 8.0 Hz, 2H), 2.74 (t, J = 7.8 Hz, 2H), 2.33-2.30 (s and m, 5H), 1.60-1.53 (m, 2H), 1.39-1.26 (m, 6H), 1.23-1.16 (m, 2H), 0.96-0.89 (m, 6H); ^{13}C NMR (CD_3OD , 100 MHz): δ = 201.9, 144.2, 140.0, 137.7, 132.2, 129.9, 129.5, 129.1, 128.2, 128.0, 127.7, 120.6, 115.5, 42.8, 33.4, 32.8, 28.4, 25.5, 23.7, 23.5, 21.4, 14.4, 14.3; HRMS m/z calcd for $\text{C}_{27}\text{H}_{34}\text{N}_2\text{O}_3\text{S}$ $[\text{M}+\text{H}]^+$: 467.2354; found: 467.2368.

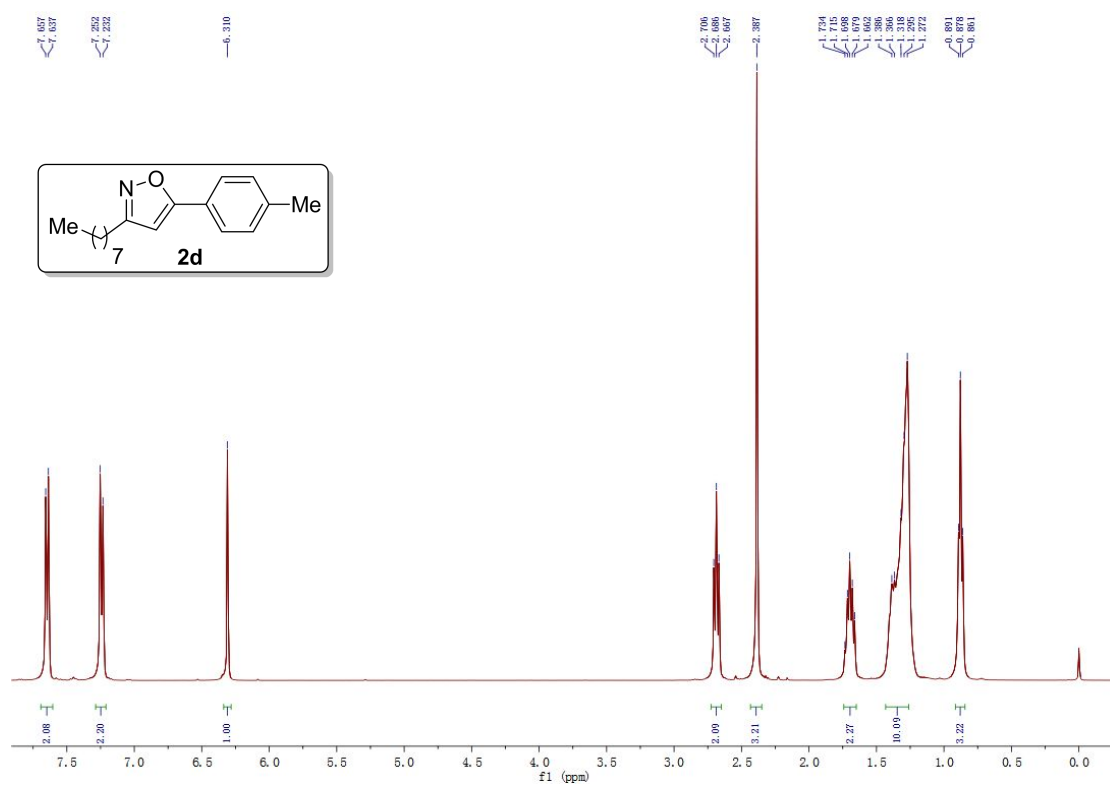


(E)-N-(4-benzoyl-2-phenyl-5-styryl-1H-pyrrol-3-yl)-4-methylbenzenesulfonamide (3z): The product was obtained as a colorless solid. (58.0 mg, 0.112 mmol), Yield: 56%; ^1H NMR (CDCl_3 , 400 MHz): δ = 8.64 (s, 1H), 7.84 (d, J = 7.2 Hz, 2H), 7.59 (s, 1H), 7.55-7.53 (m, 1H), 7.43-7.39 (m, 4H), 7.36-7.29 (m, 5H), 7.21-7.19 (m, 3H), 7.01 (d, J = 7.2 Hz, 2H), 6.86 (d, J = 7.6 Hz, 2H), 6.68 (d, J = 16.4 Hz, 1H), 6.30 (d, J = 16.8 Hz, 1H), 2.03 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): δ =

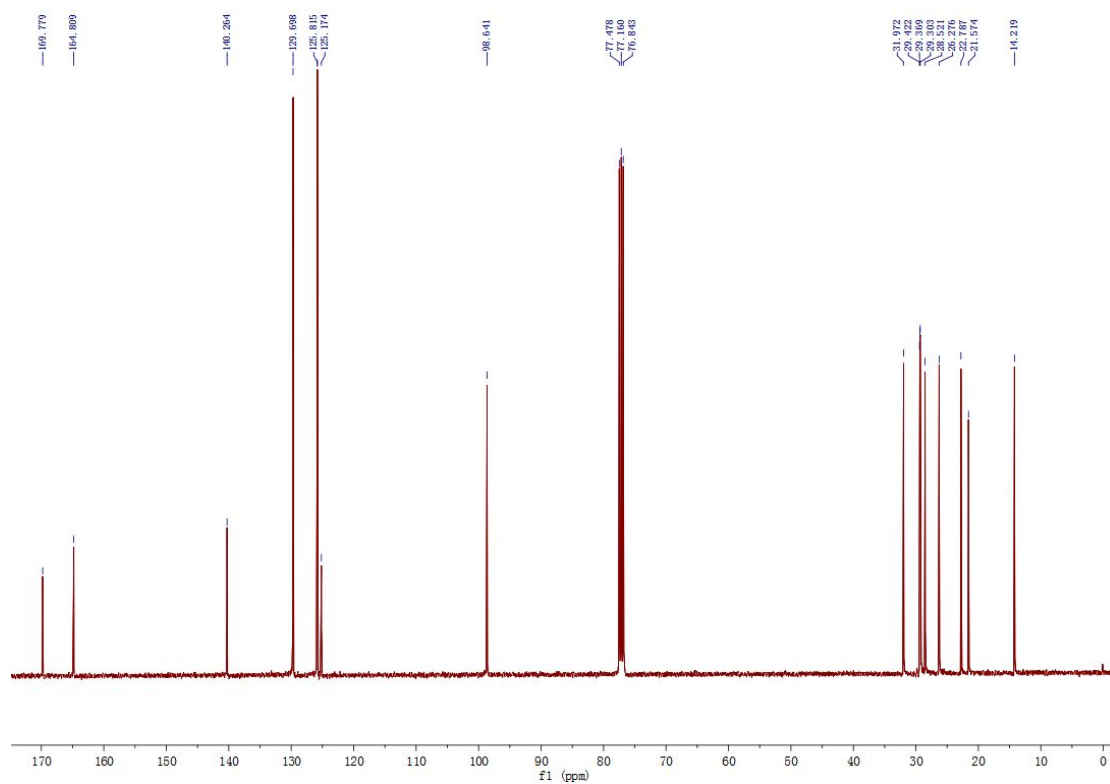
192.1, 143.4, 138.8, 136.1, 135.1, 132.5, 132.2, 130.5, 130.3, 129.8, 129.4, 128.9, 128.9, 128.3, 128.2, 128.0, 128.0, 127.8, 126.8, 126.3, 119.8, 118.9, 116.9, 21.4; HRMS m/z calcd for $C_{32}H_{26}N_2O_3S$ $[M+H]^+$: 519.1740; found: 519.1742.

7. NMR Spectra of Isoxazoles

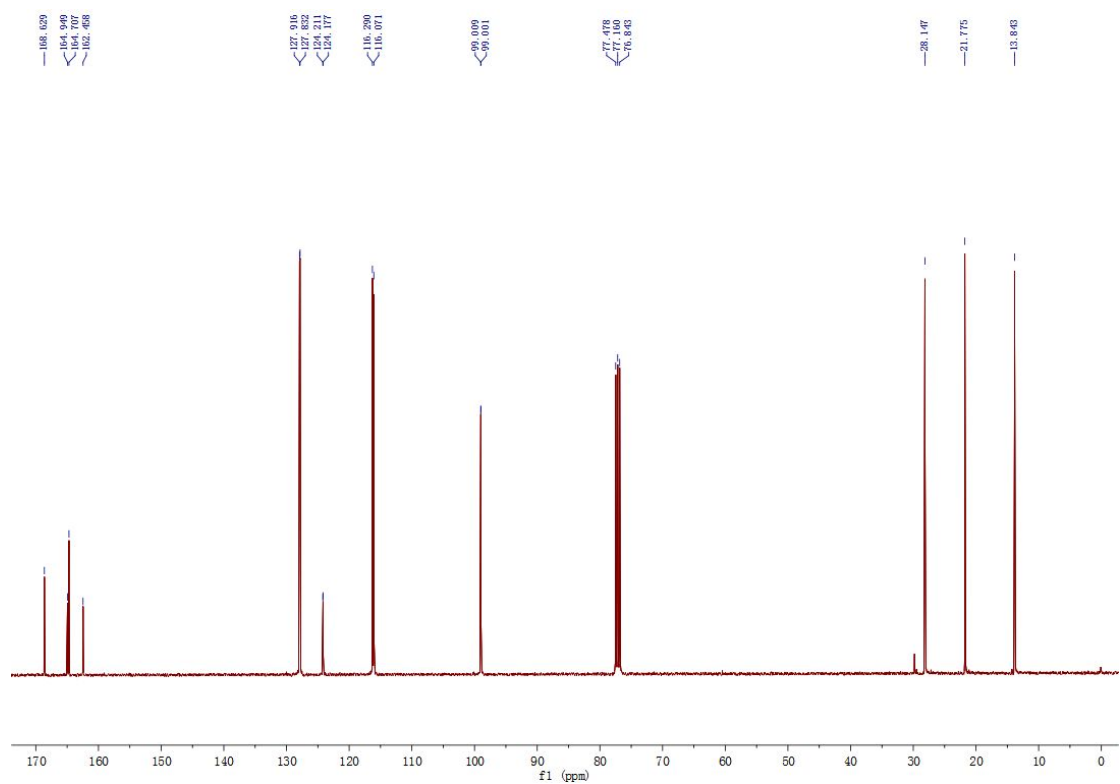
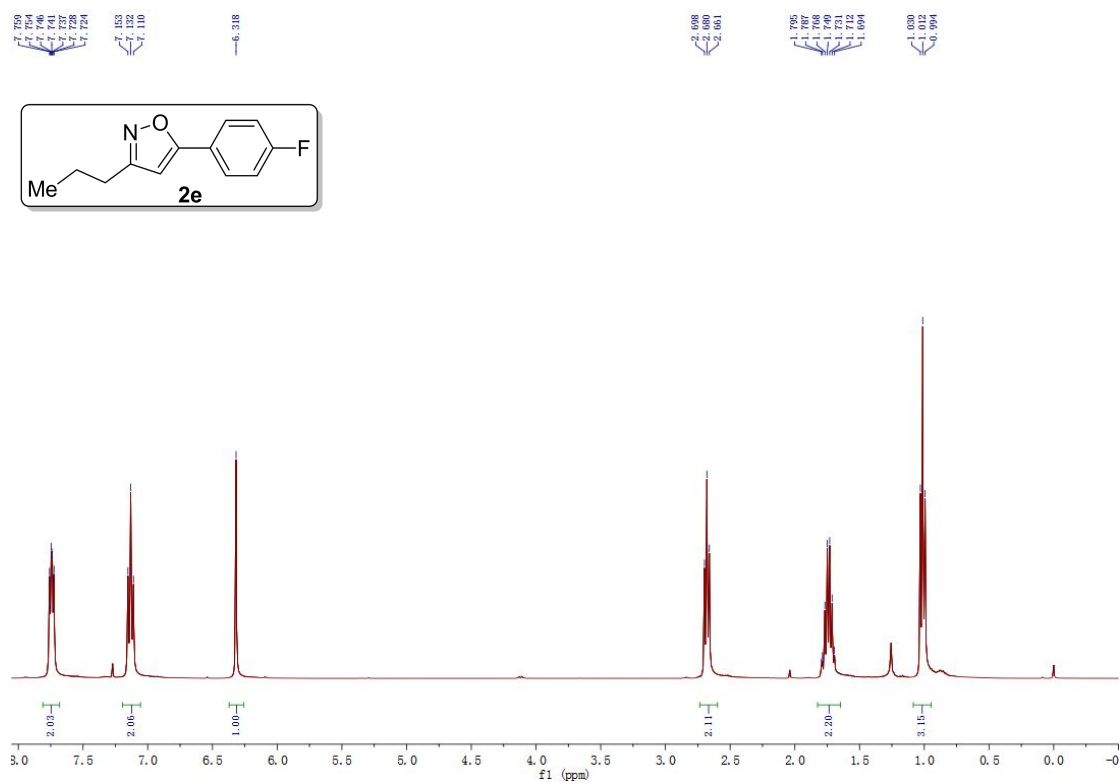


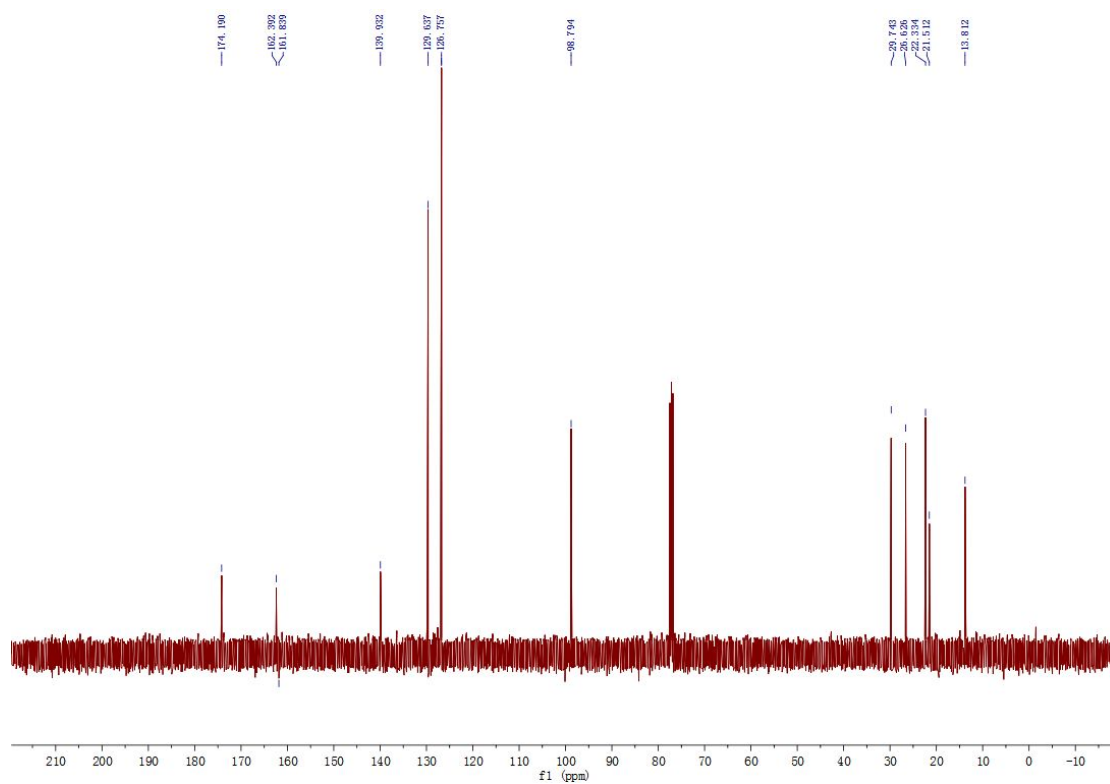
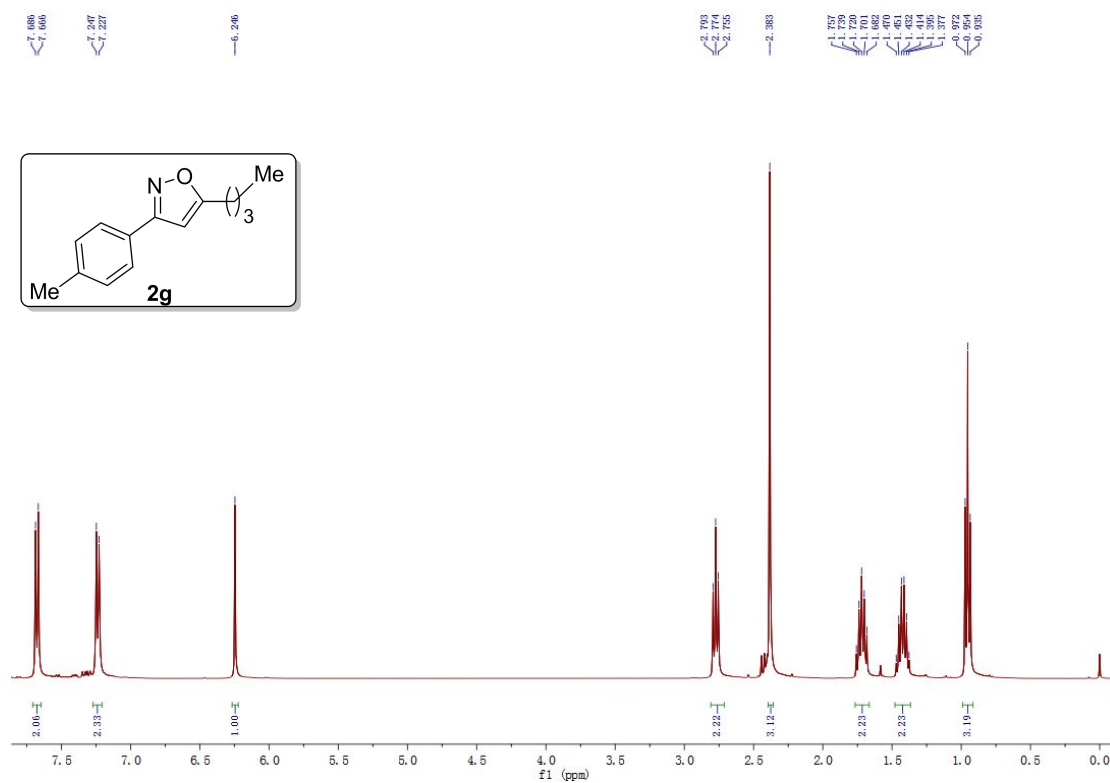


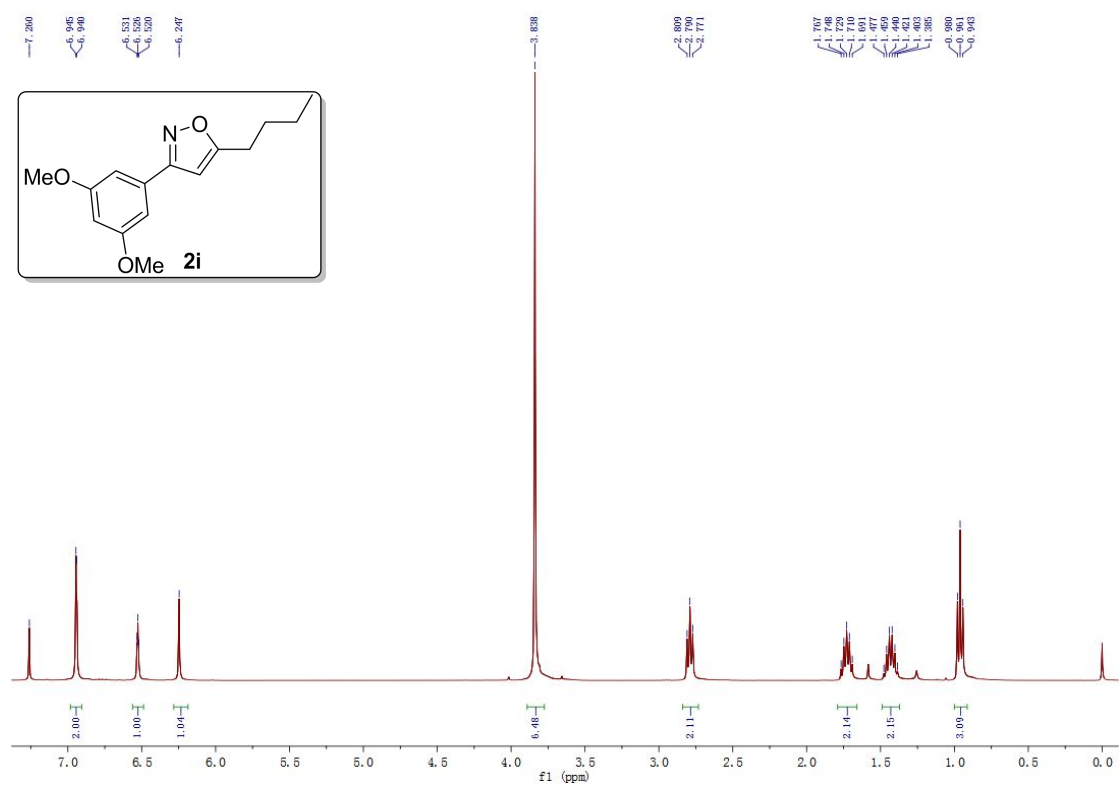
¹H NMR Spectrum for **2d** (CDCl₃, 400 MHz)



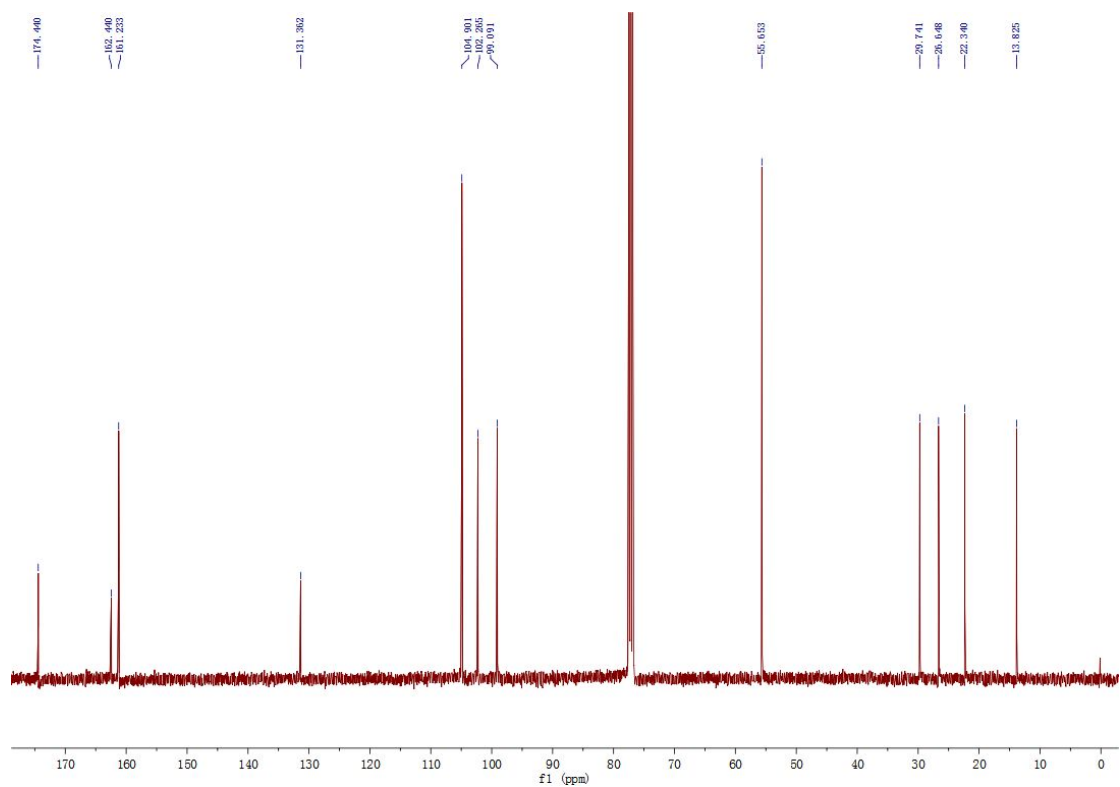
¹³C NMR Spectrum for **2d** (CDCl₃, 100 MHz)



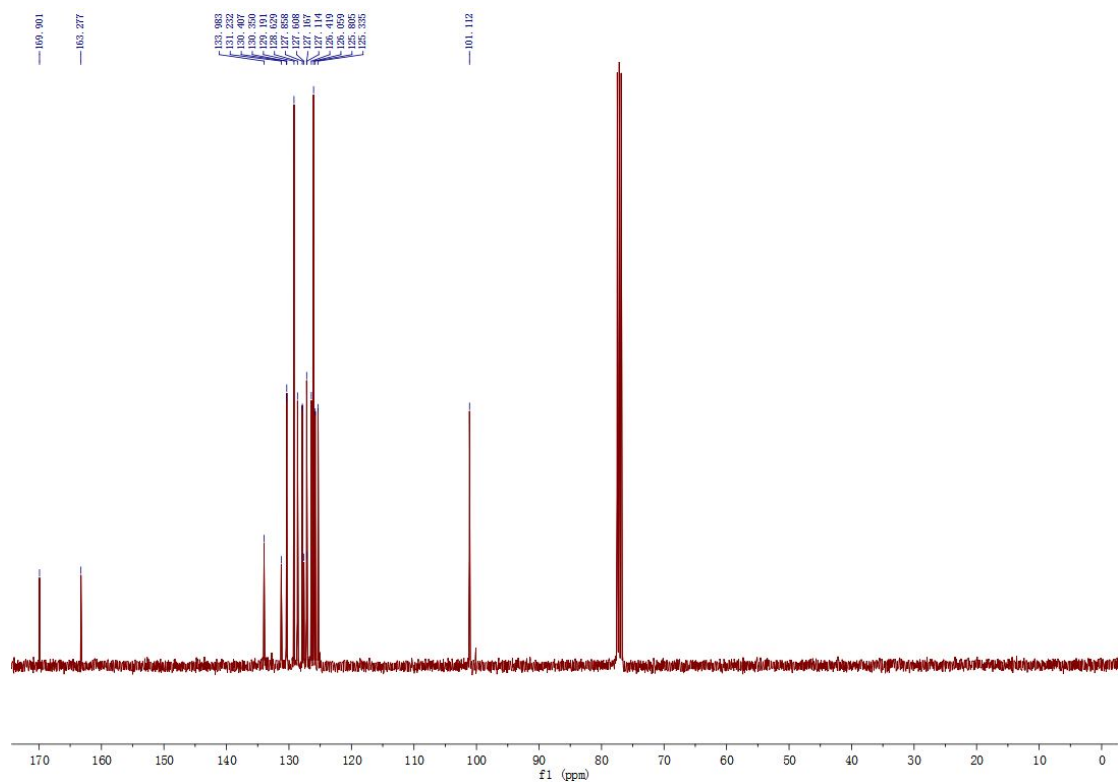
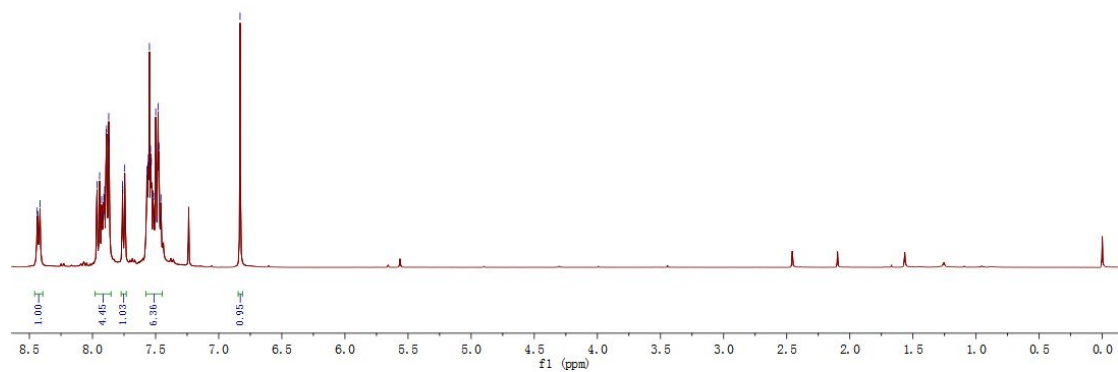
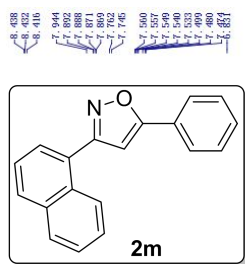




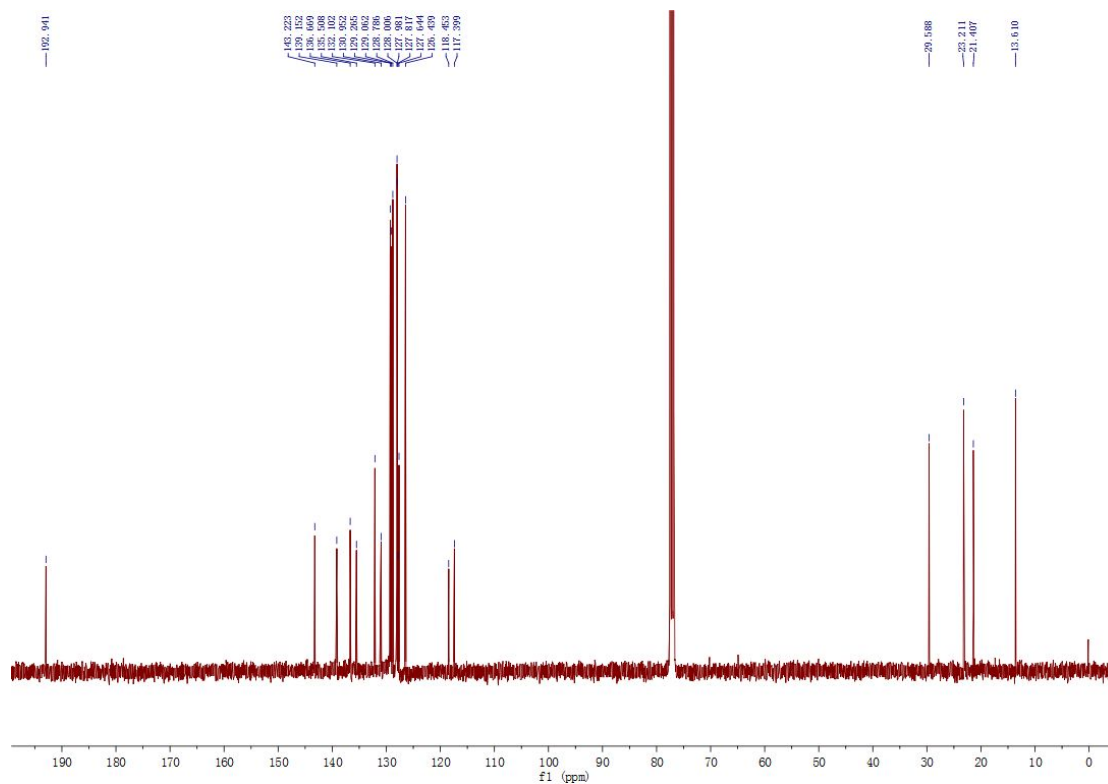
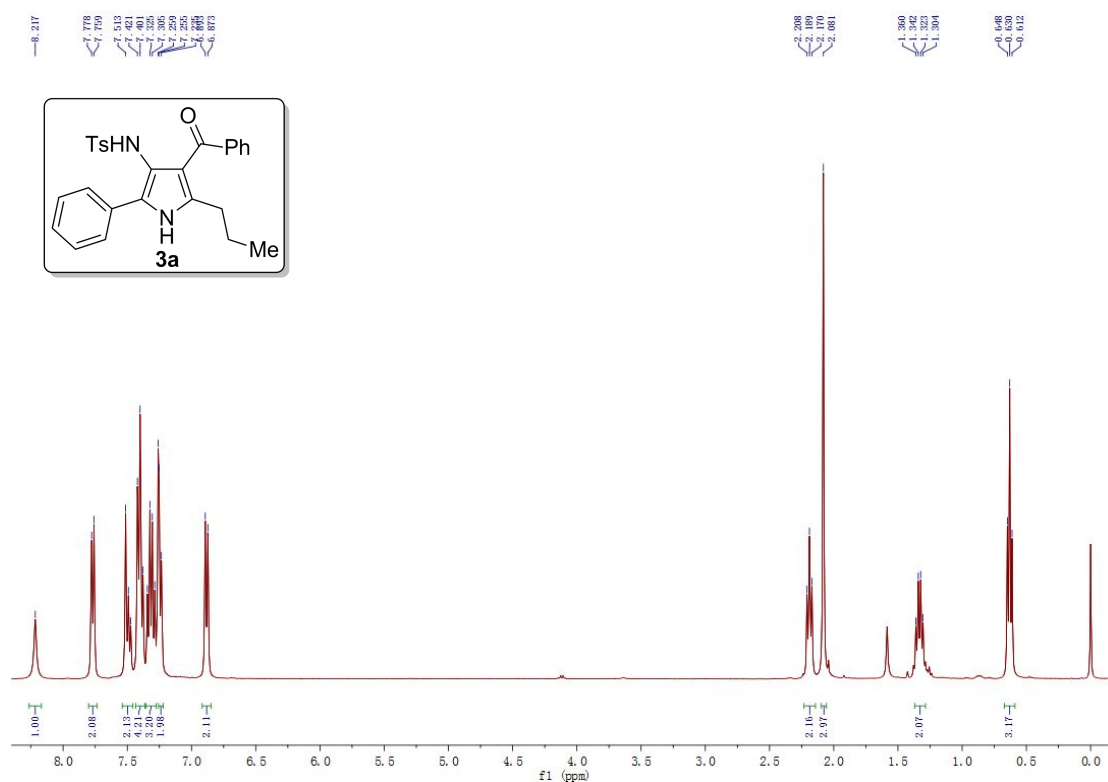
¹H NMR Spectrum for **2i** (CDCl₃, 400 MHz)

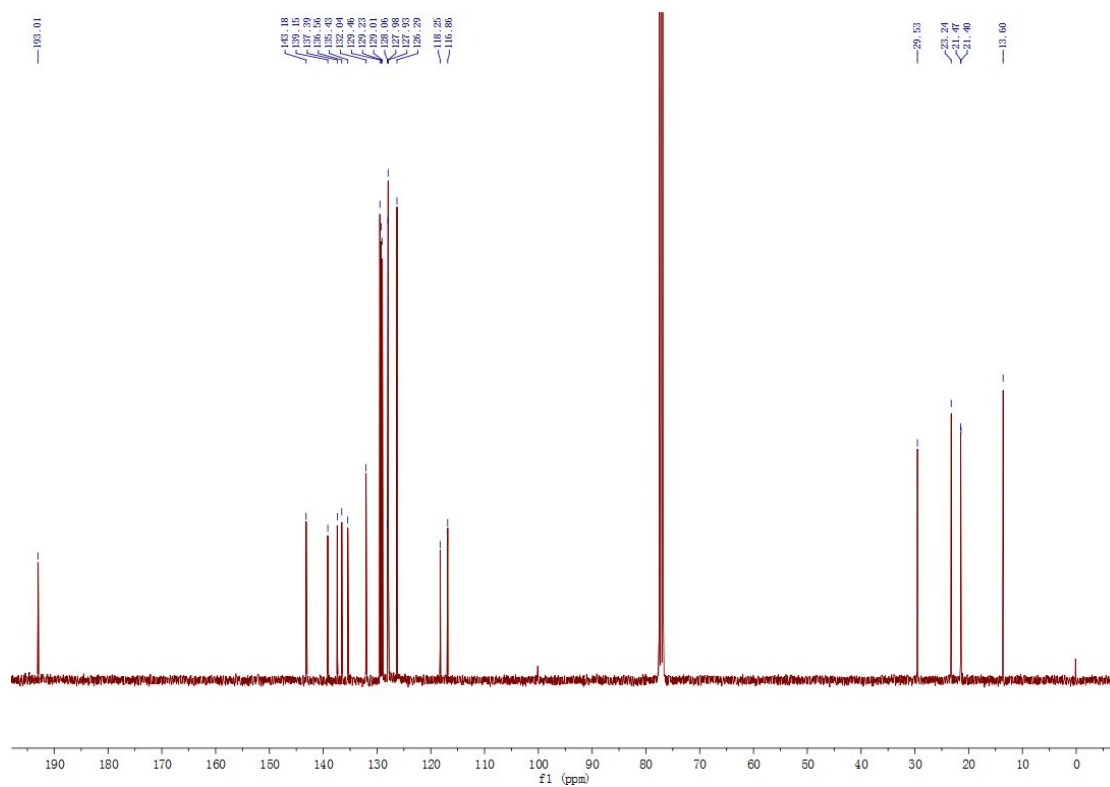
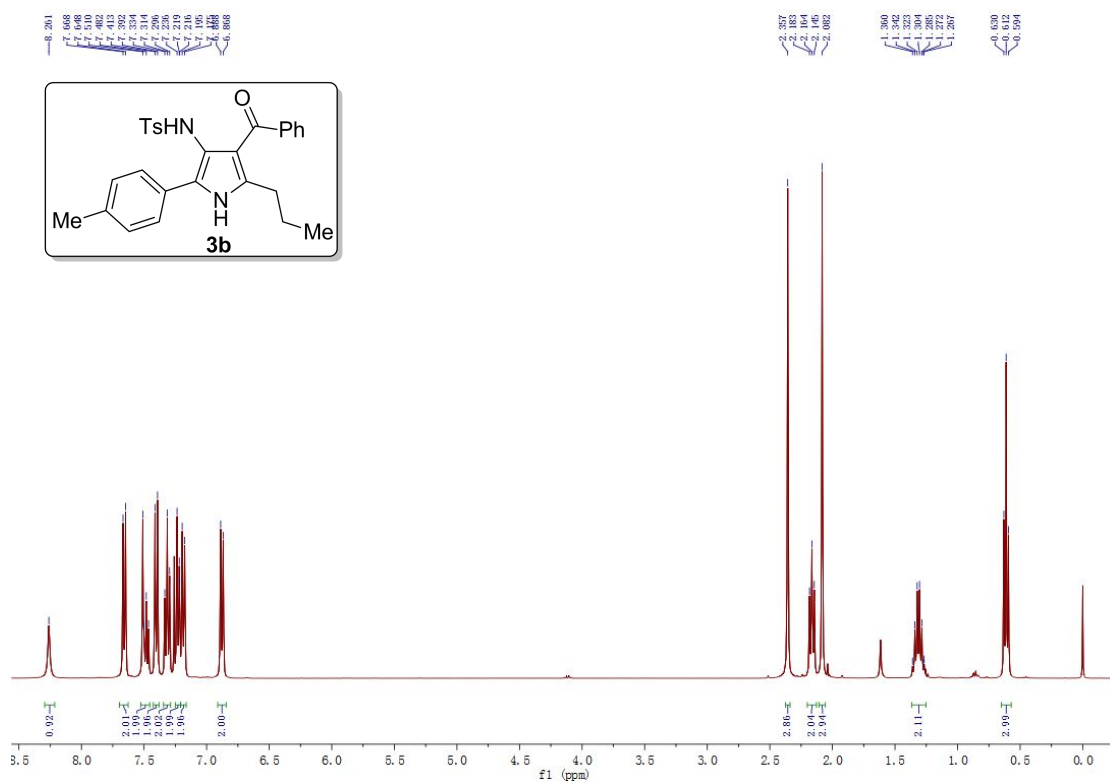


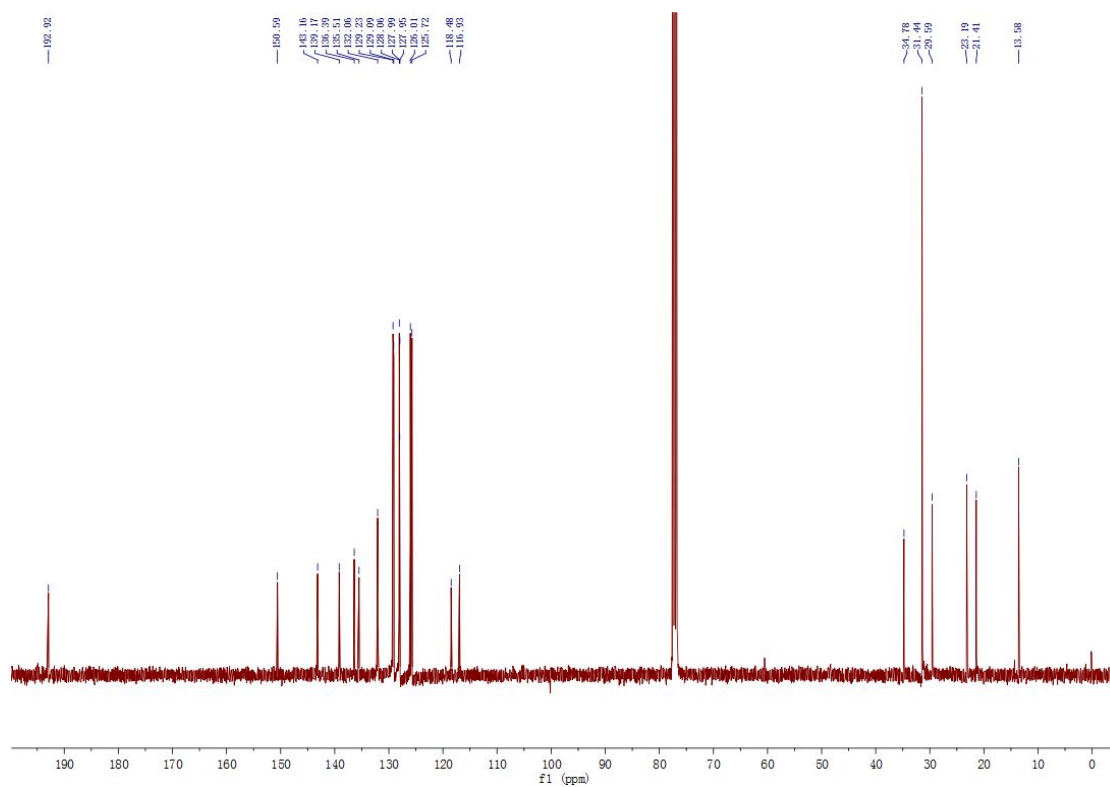
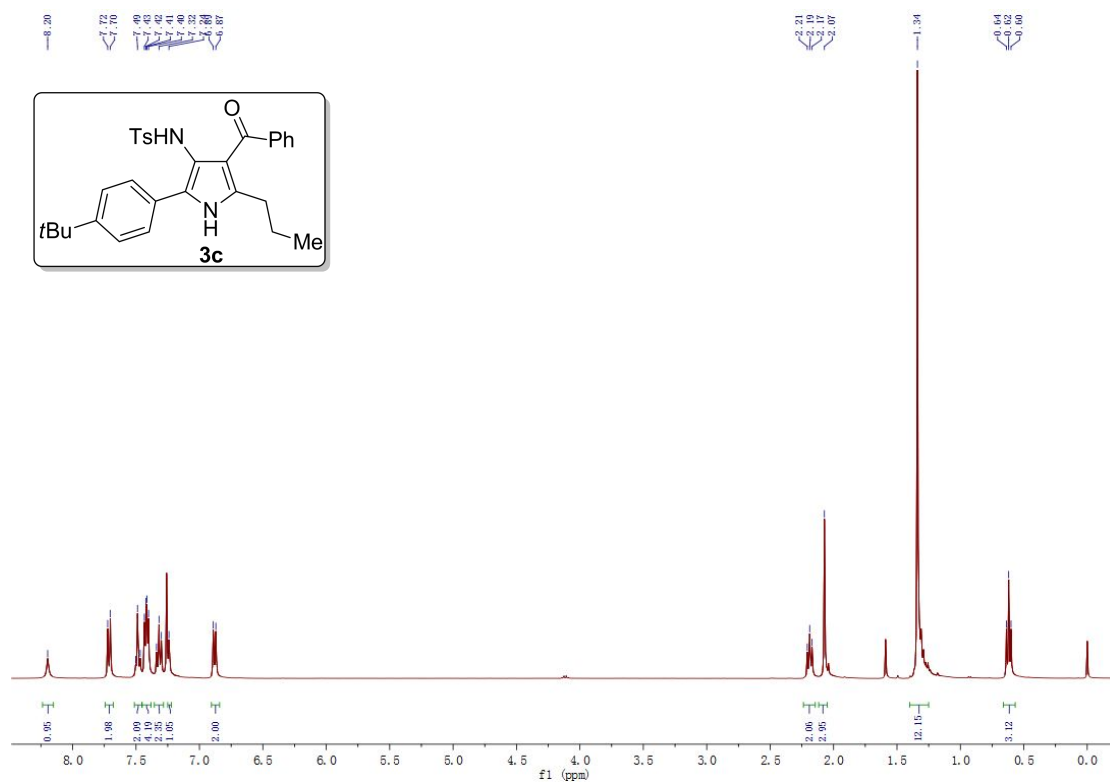
¹³C NMR Spectrum for **2i** (CDCl₃, 100 MHz)

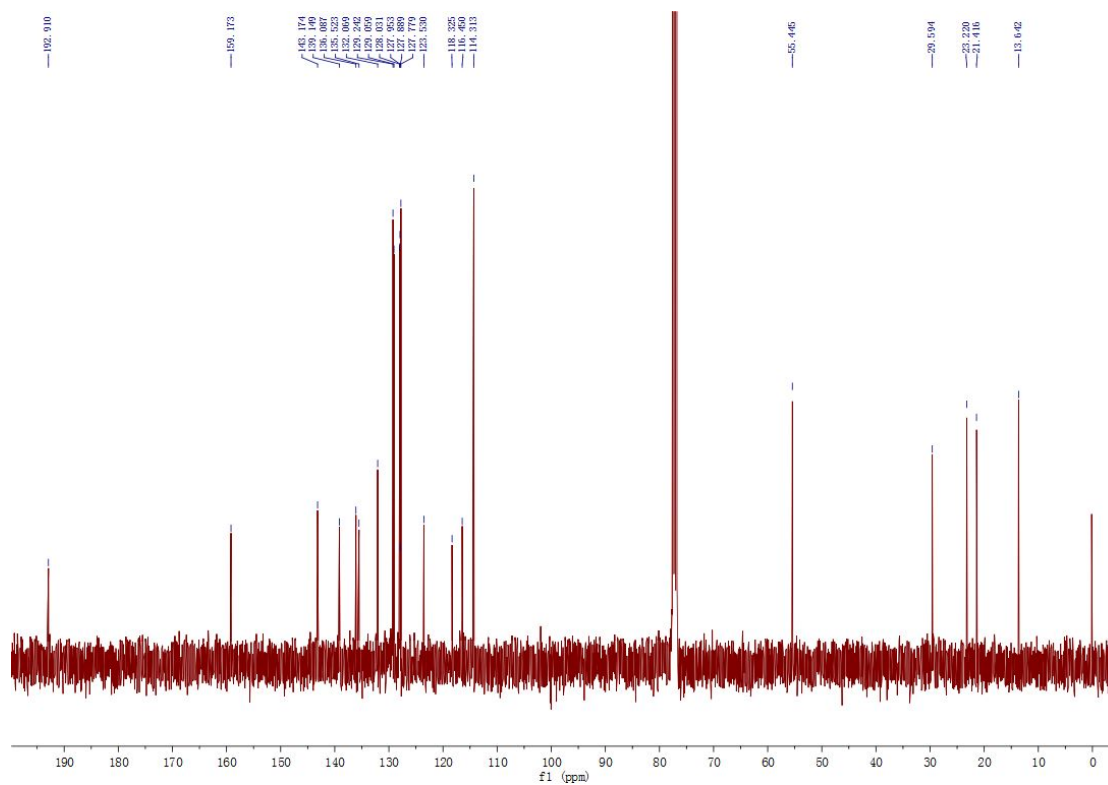
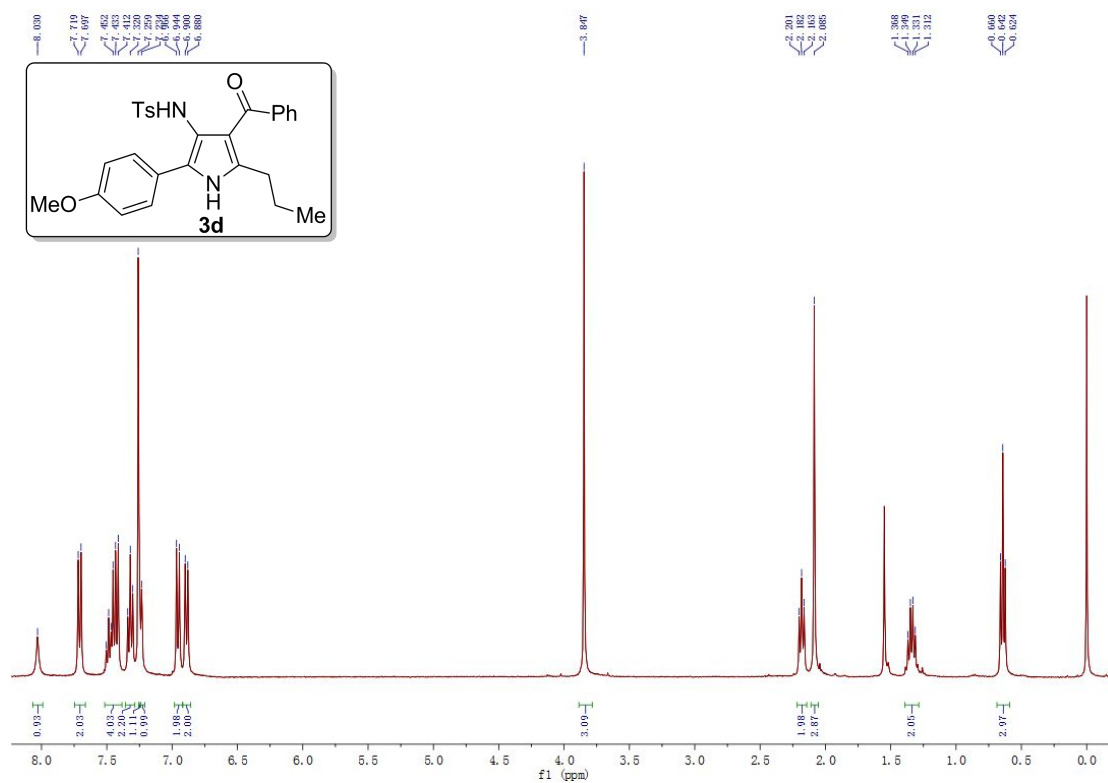


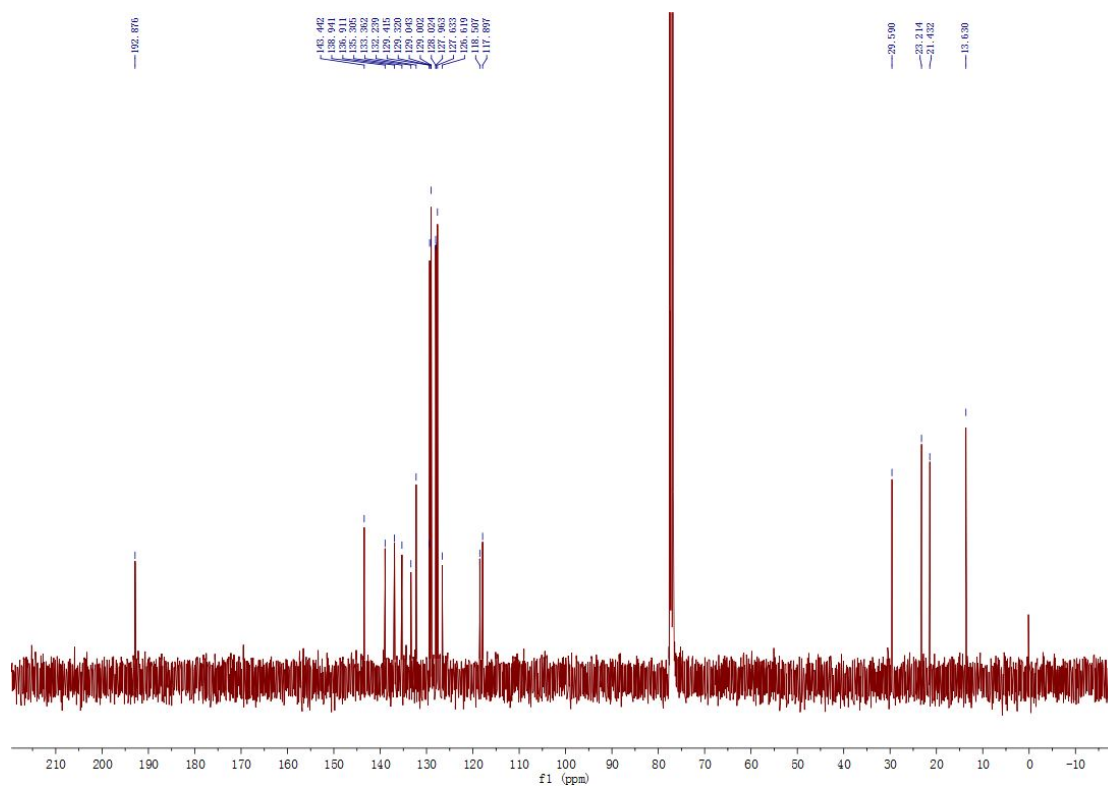
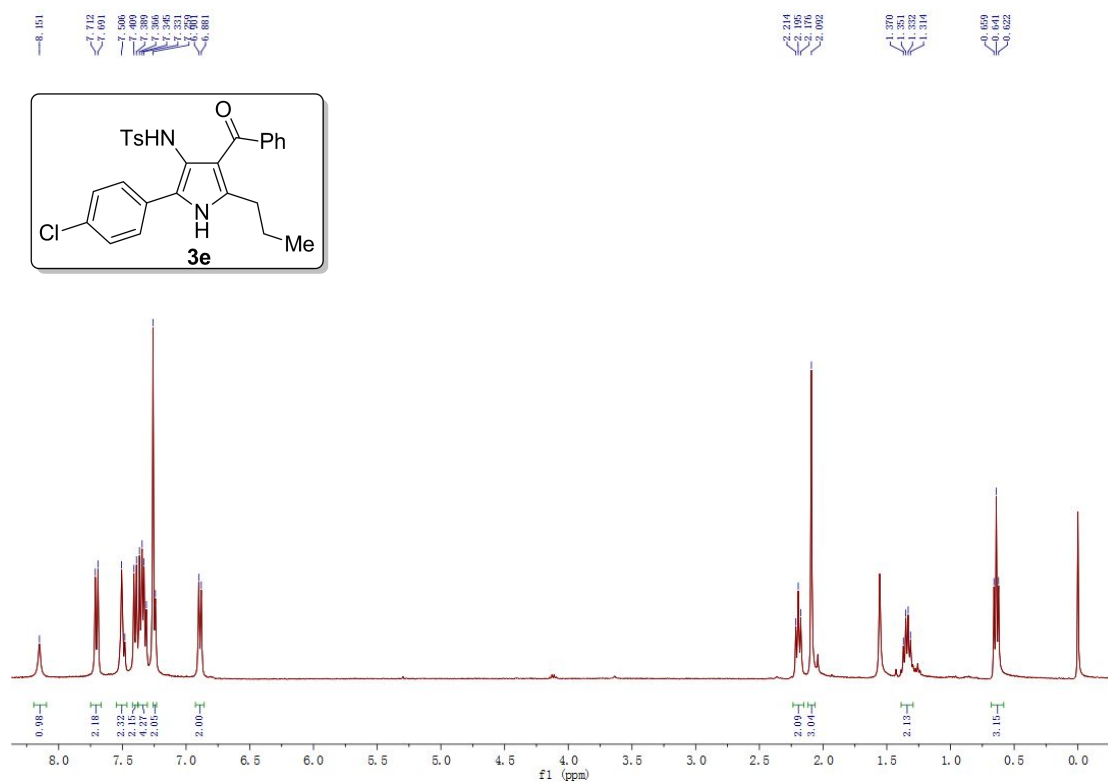
8. NMR Spectra of 3-Aminopyrroles

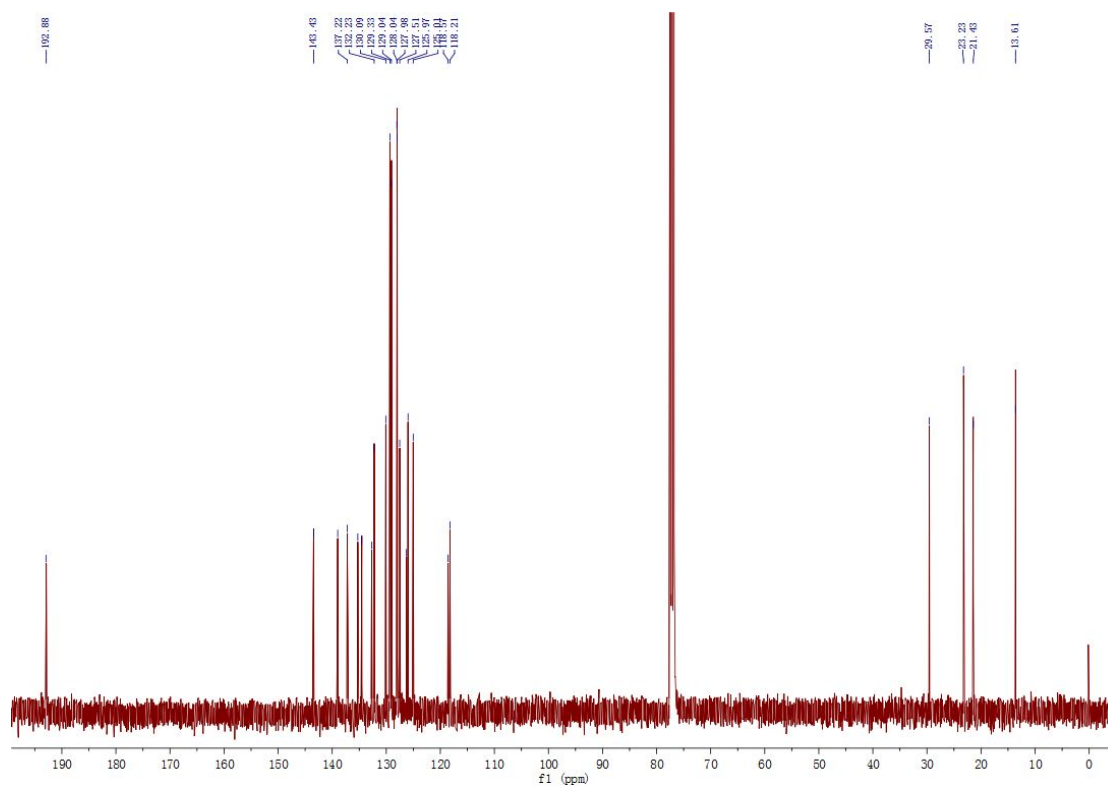
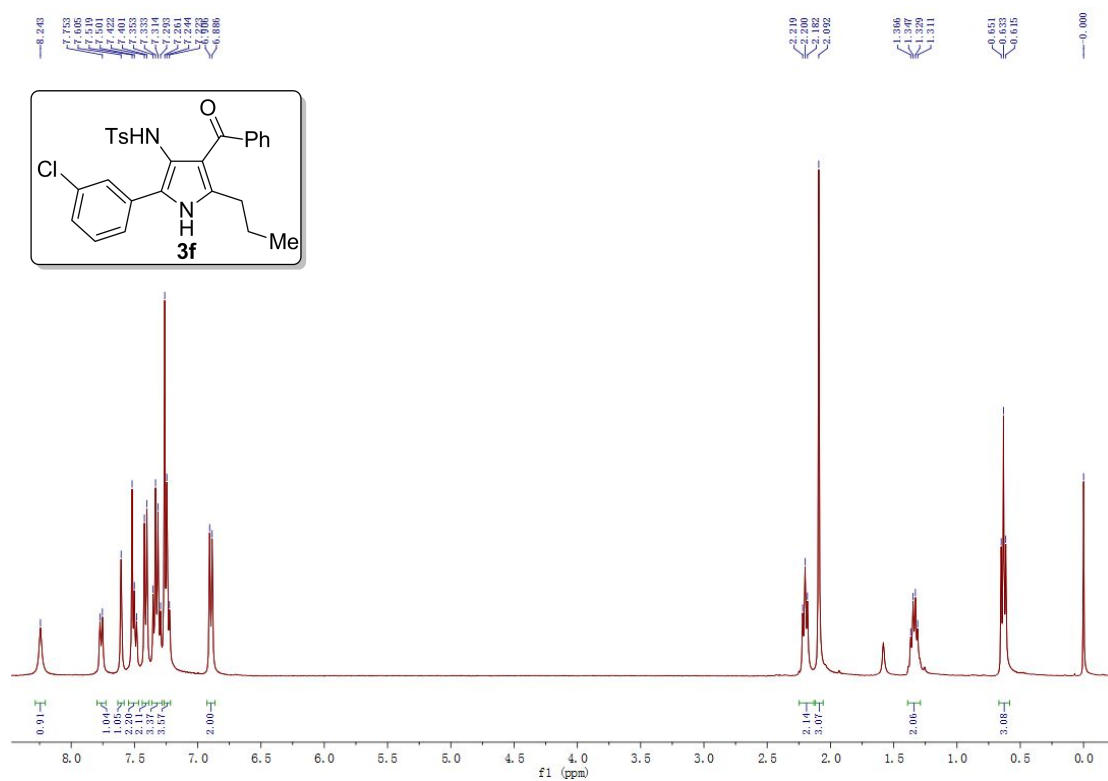


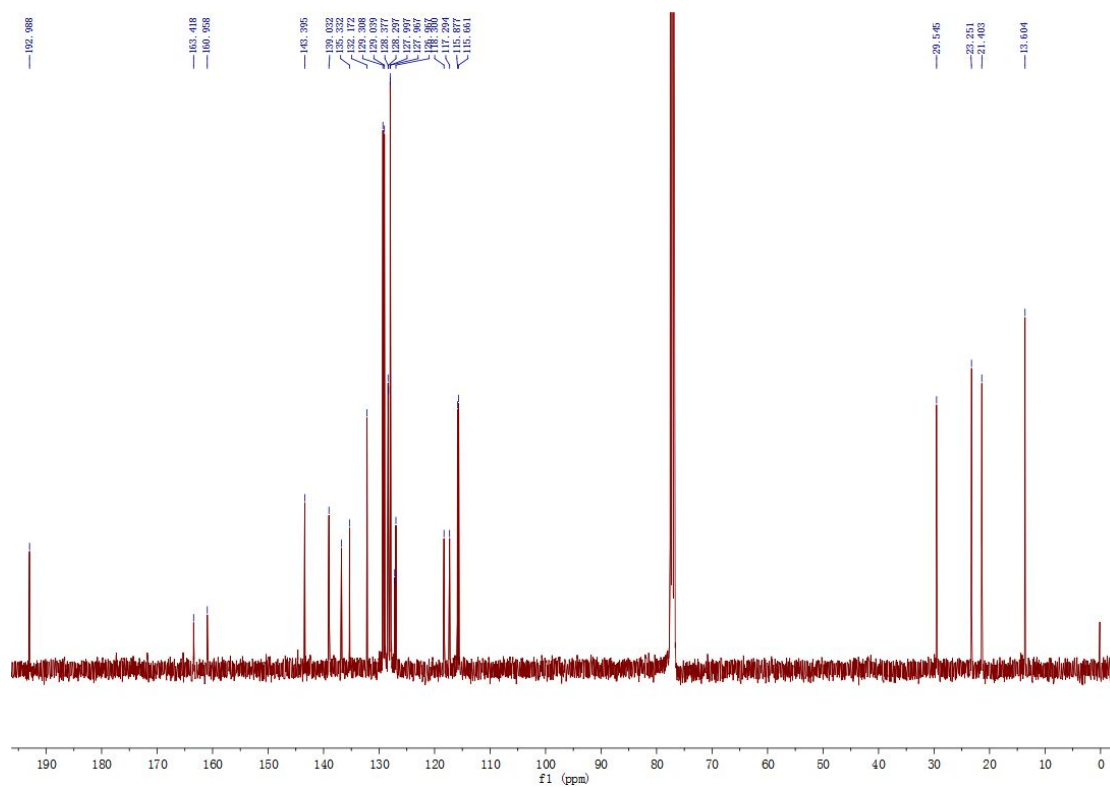
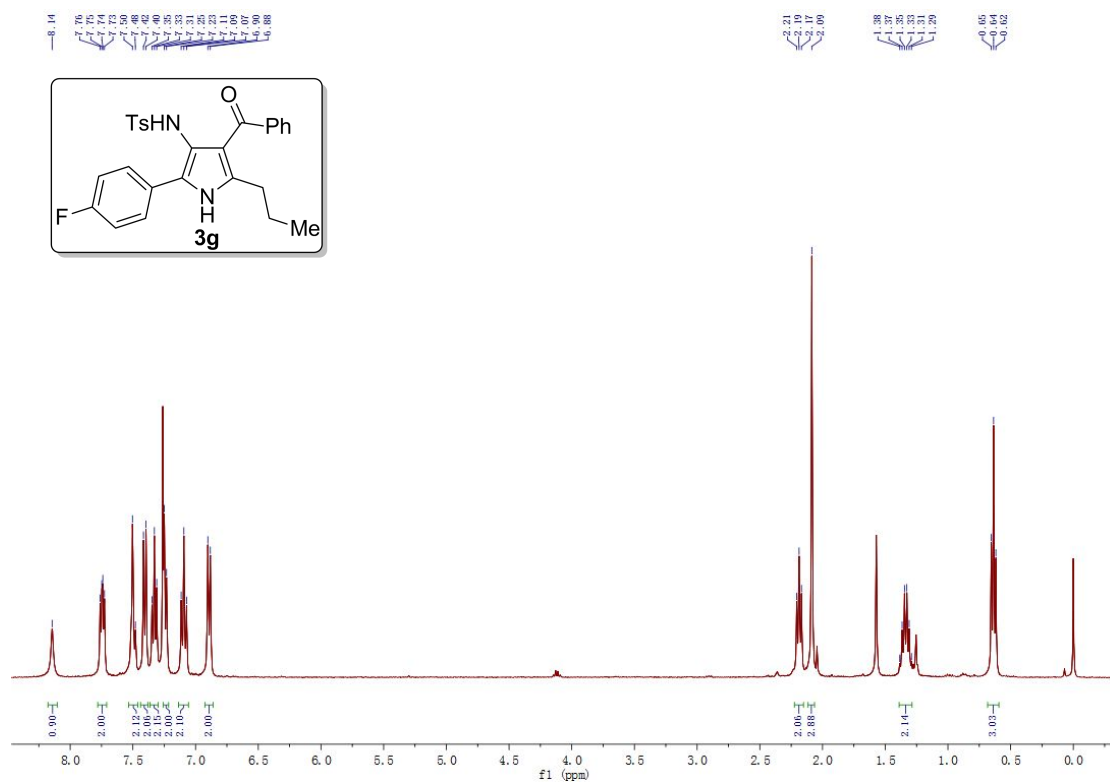


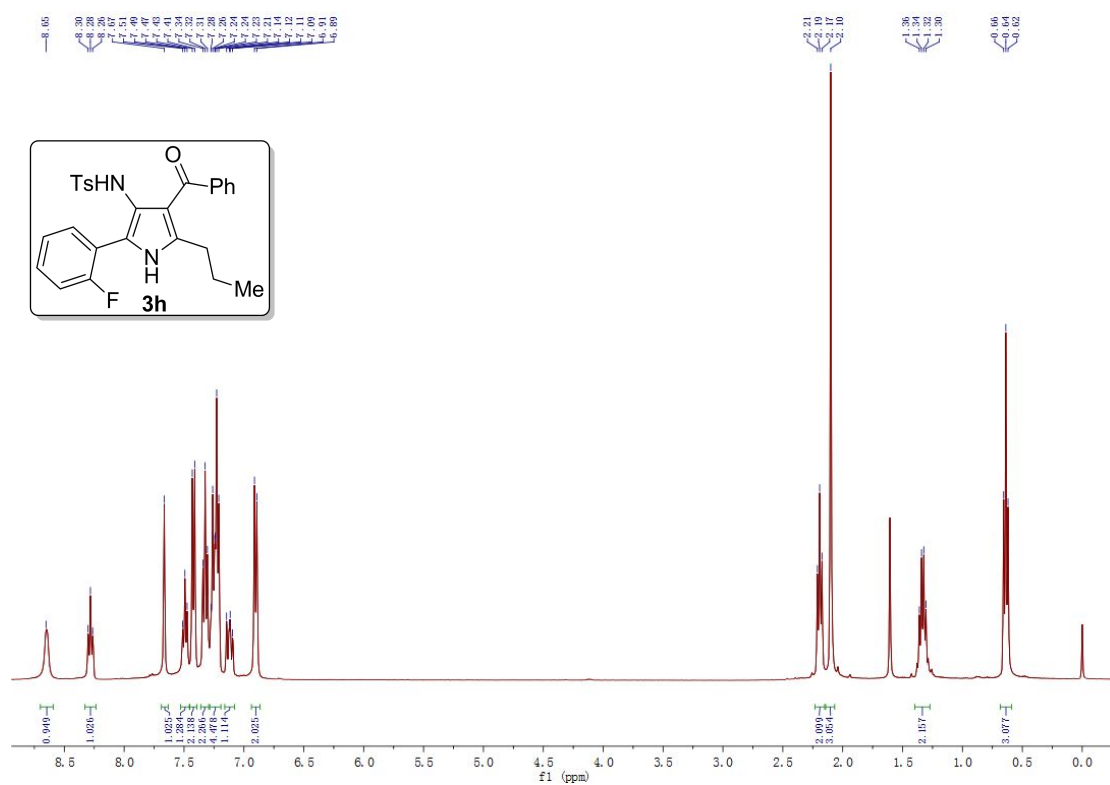




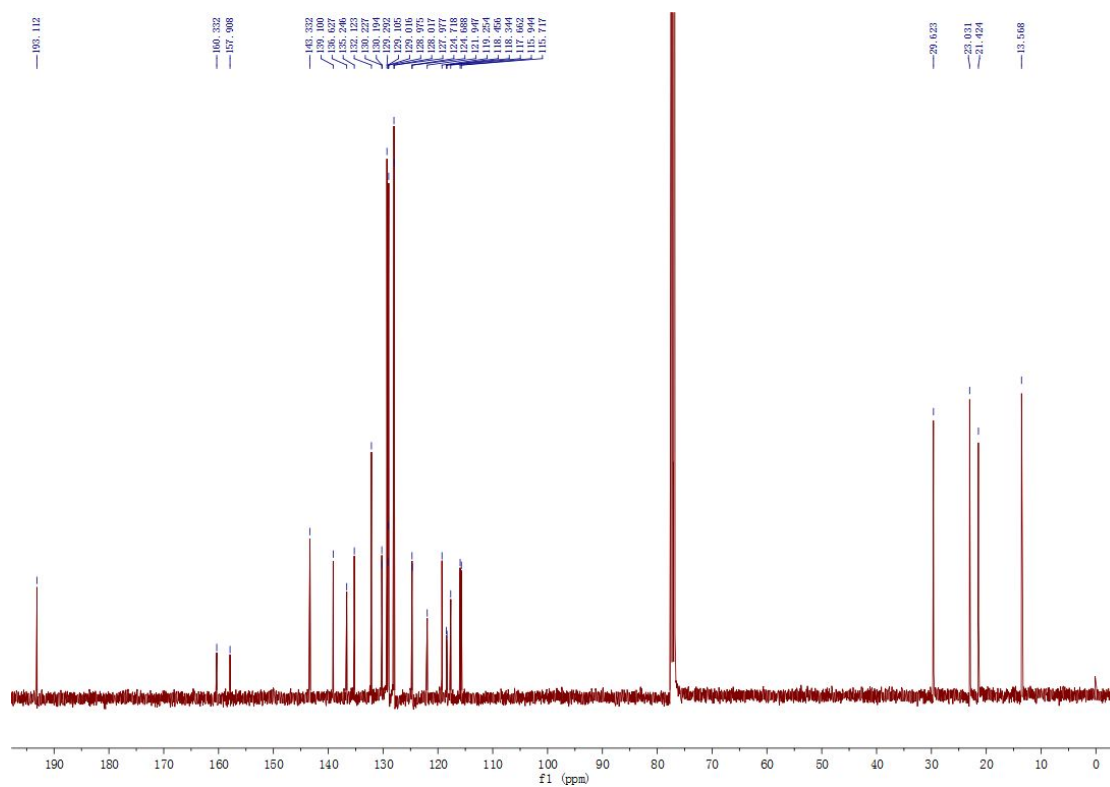




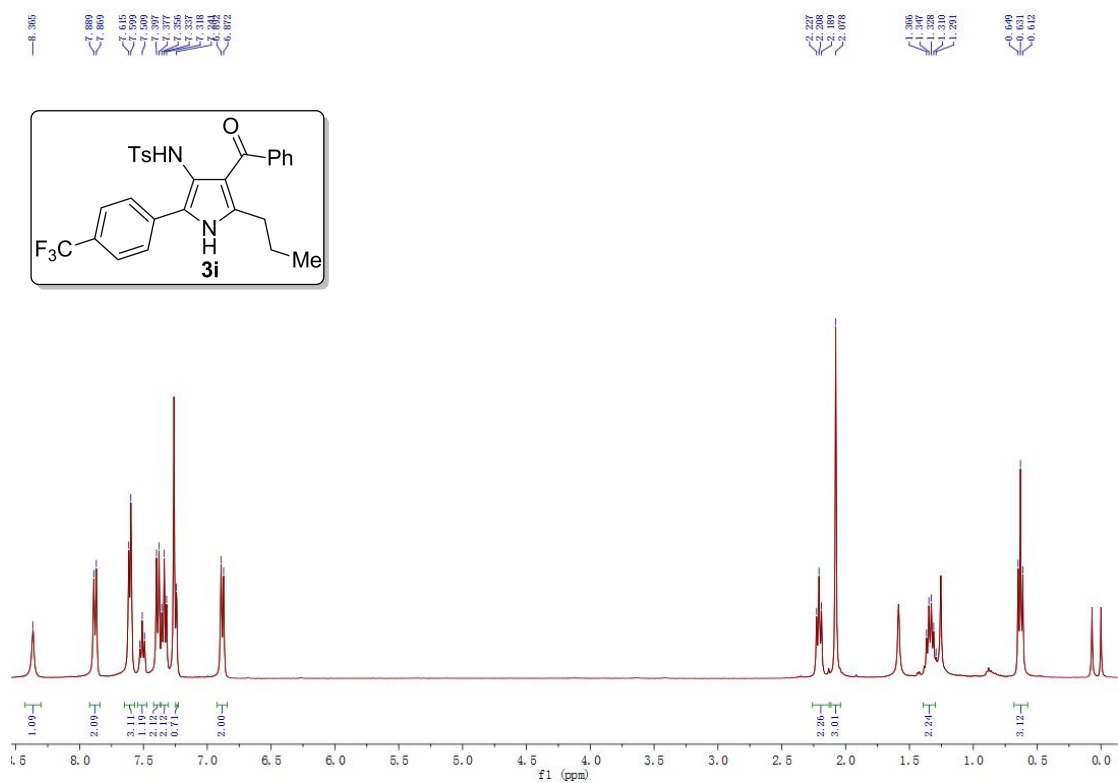




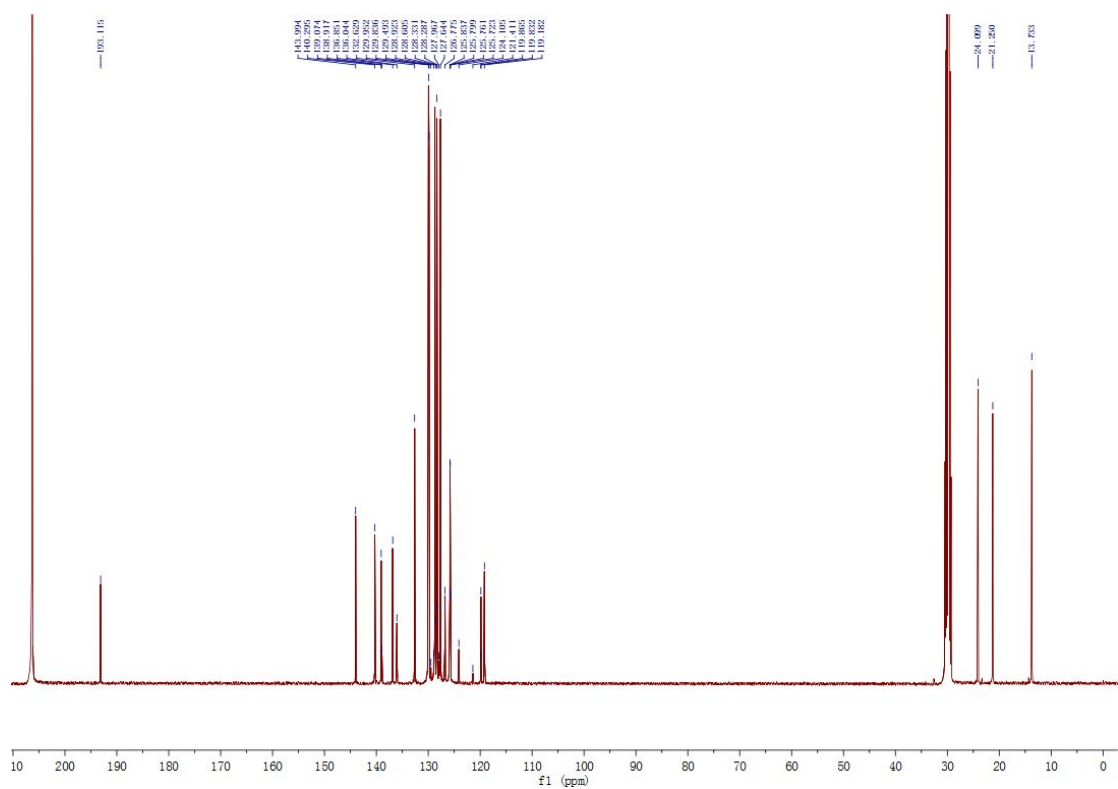
¹H NMR Spectrum for **3h** (CDCl₃, 400 MHz)



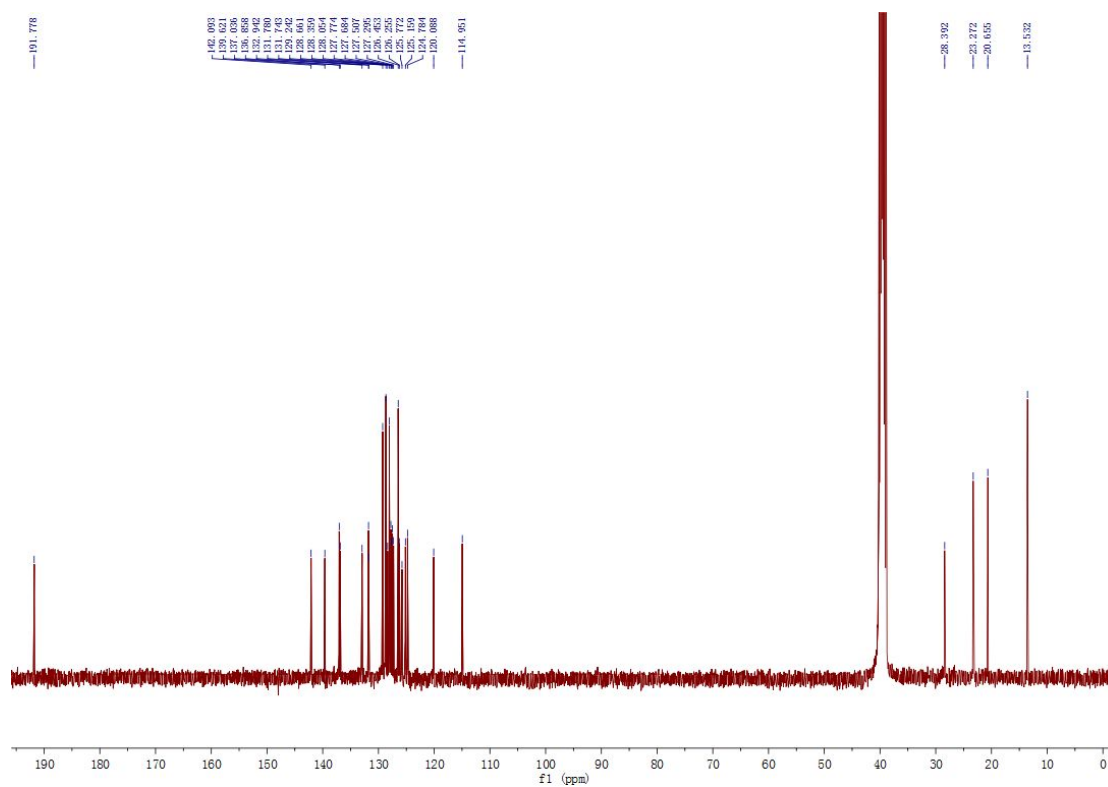
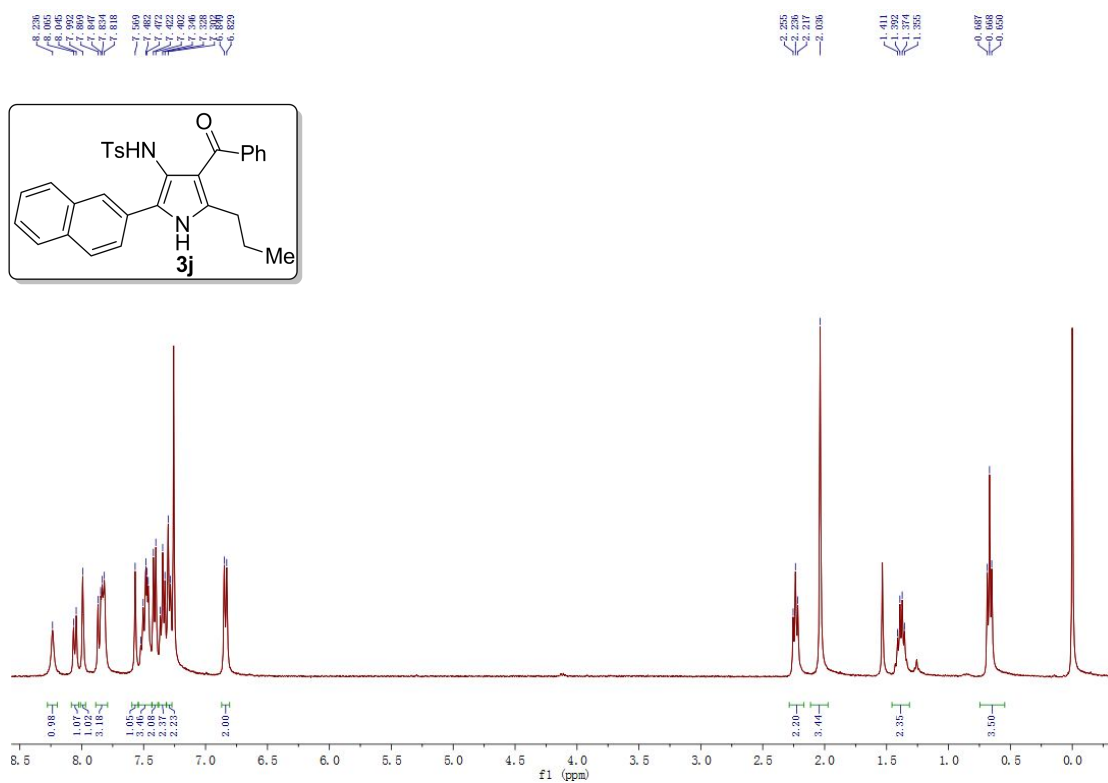
¹³C NMR Spectrum for **3h** (CDCl₃, 100 MHz)

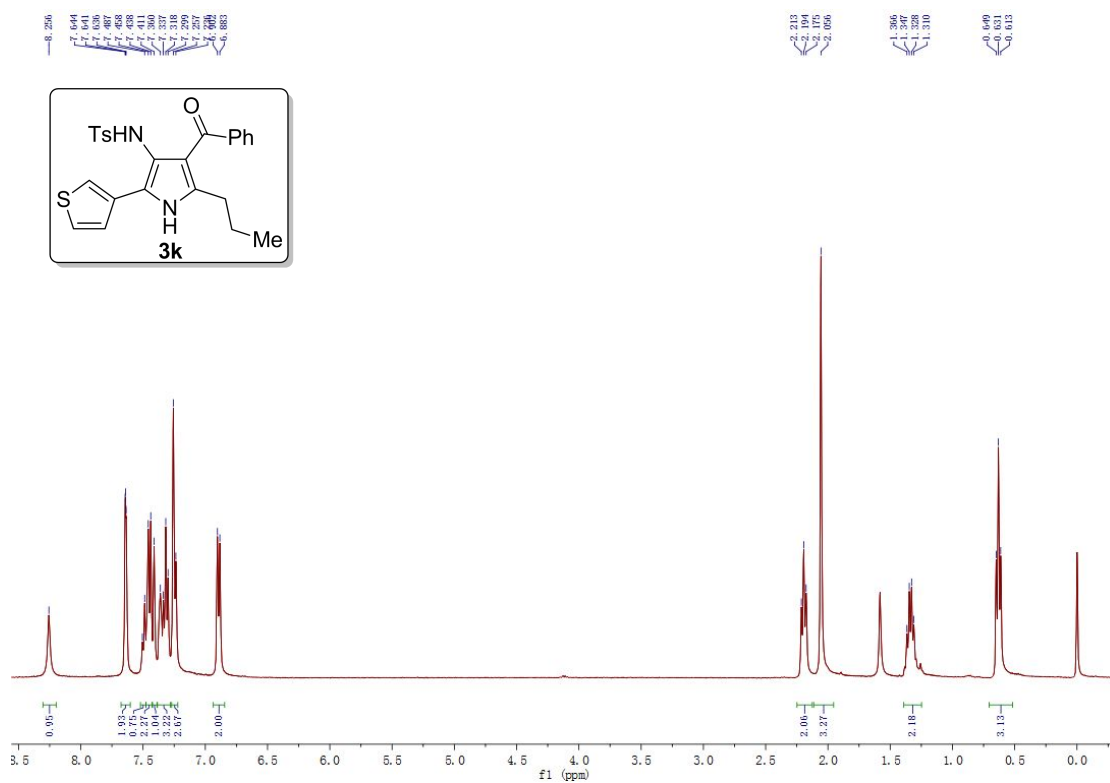


¹H NMR Spectrum for **3i** (CDCl₃, 400 MHz)

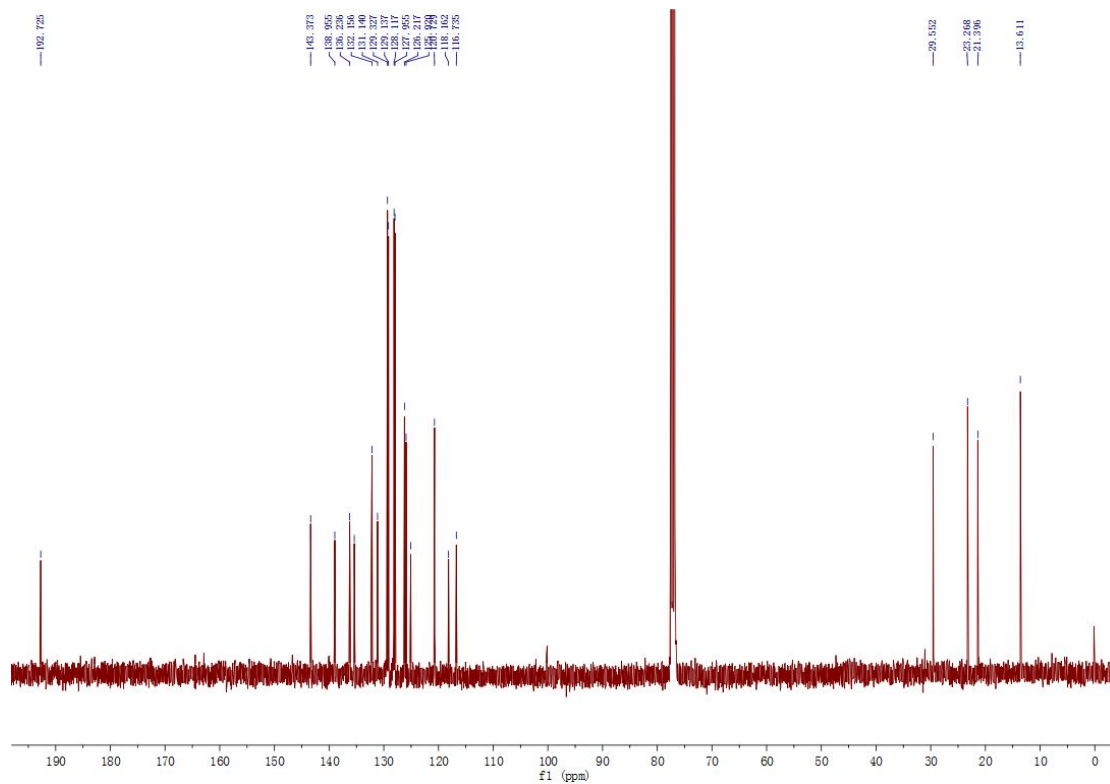


¹³C NMR Spectrum for **3i** (CDCl₃, 100 MHz)

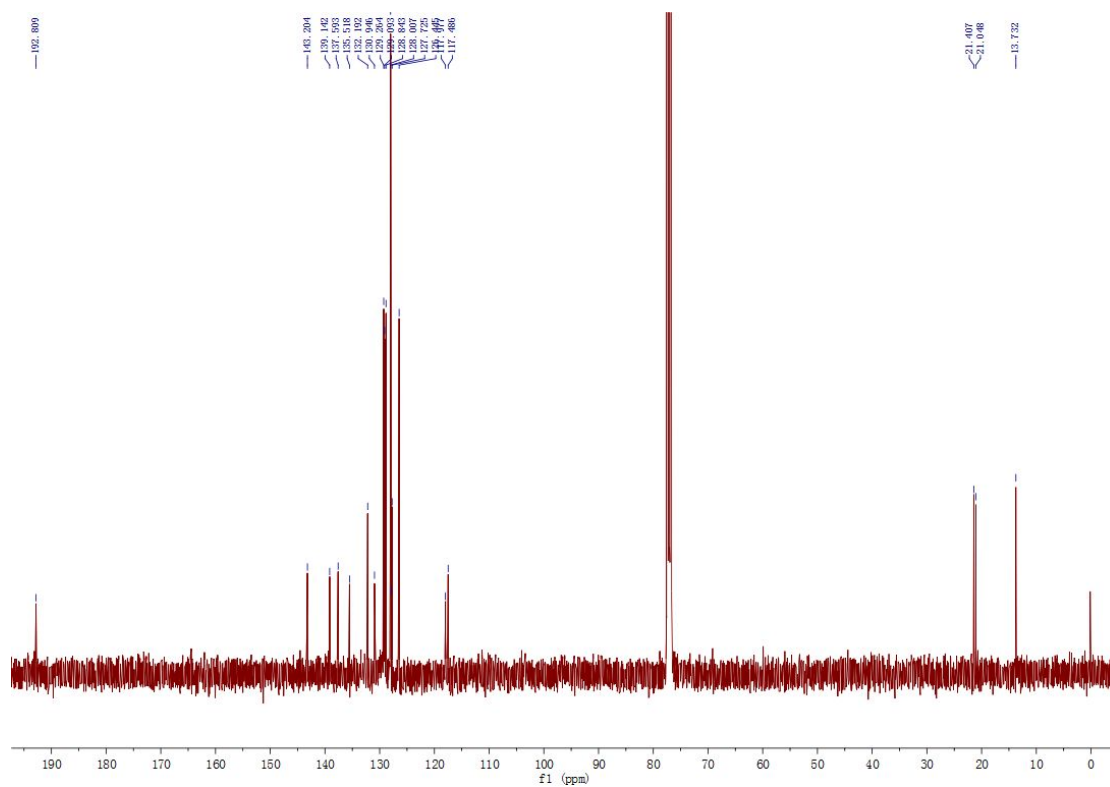
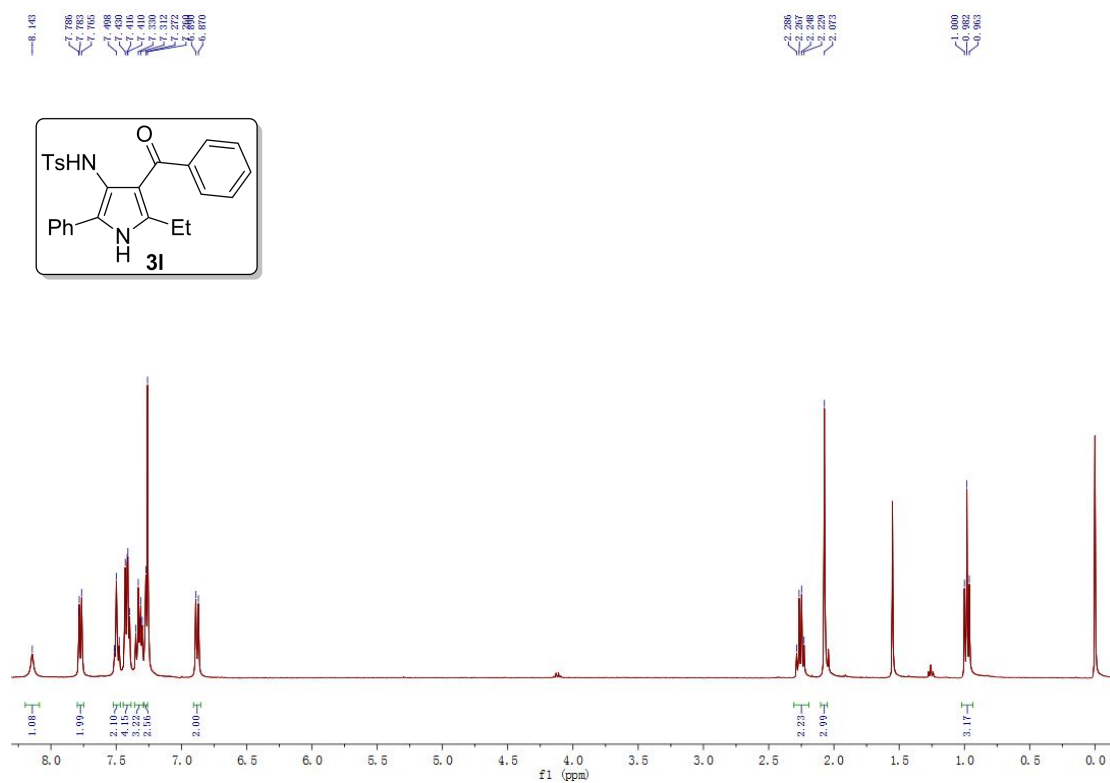


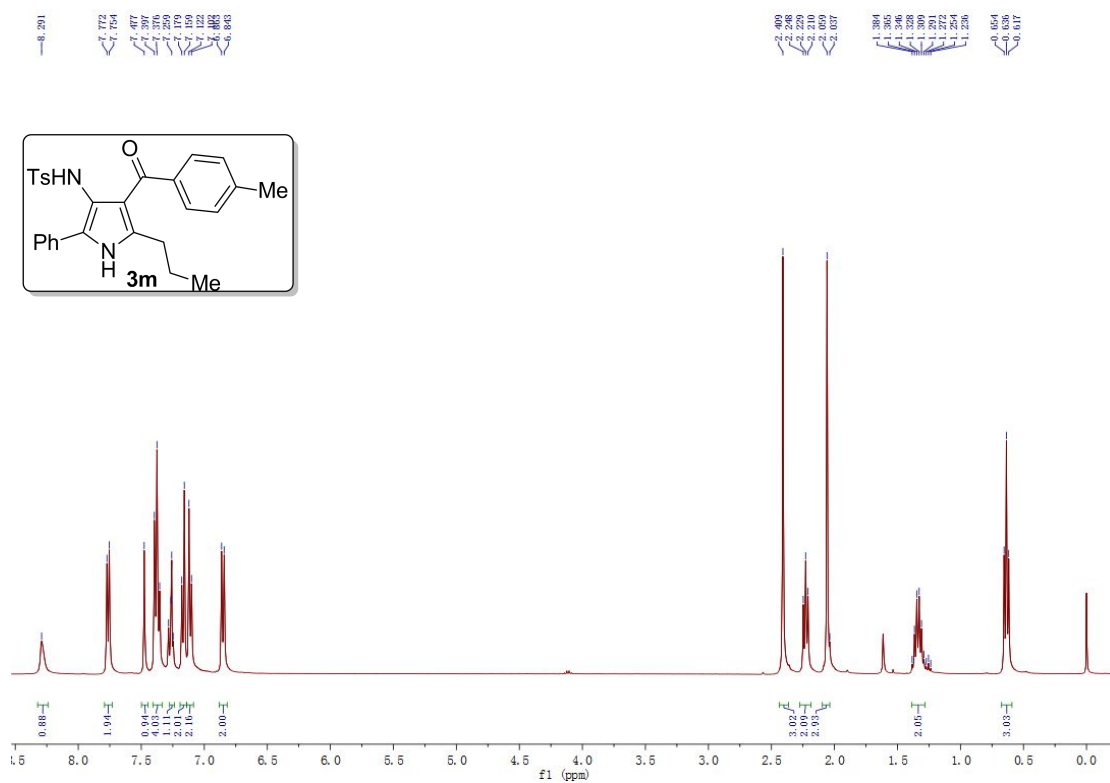


¹H NMR Spectrum for **3k** (CDCl₃, 400 MHz)

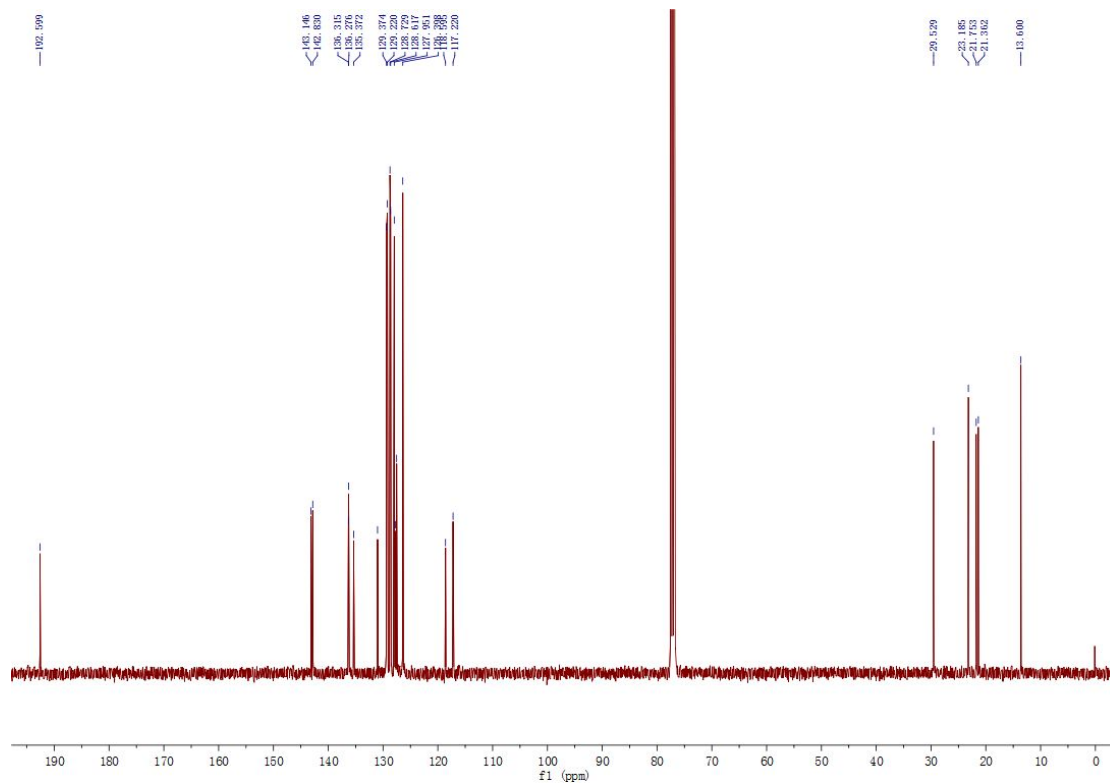


¹³C NMR Spectrum for **3k** (CDCl₃, 100 MHz)

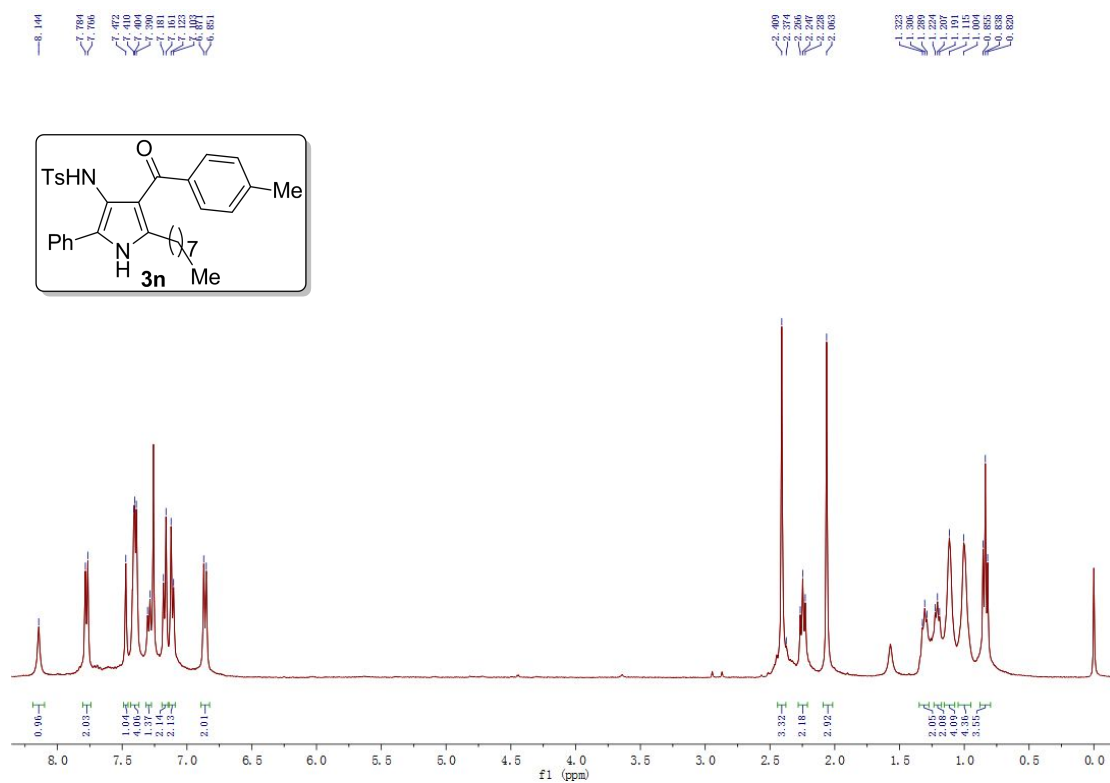




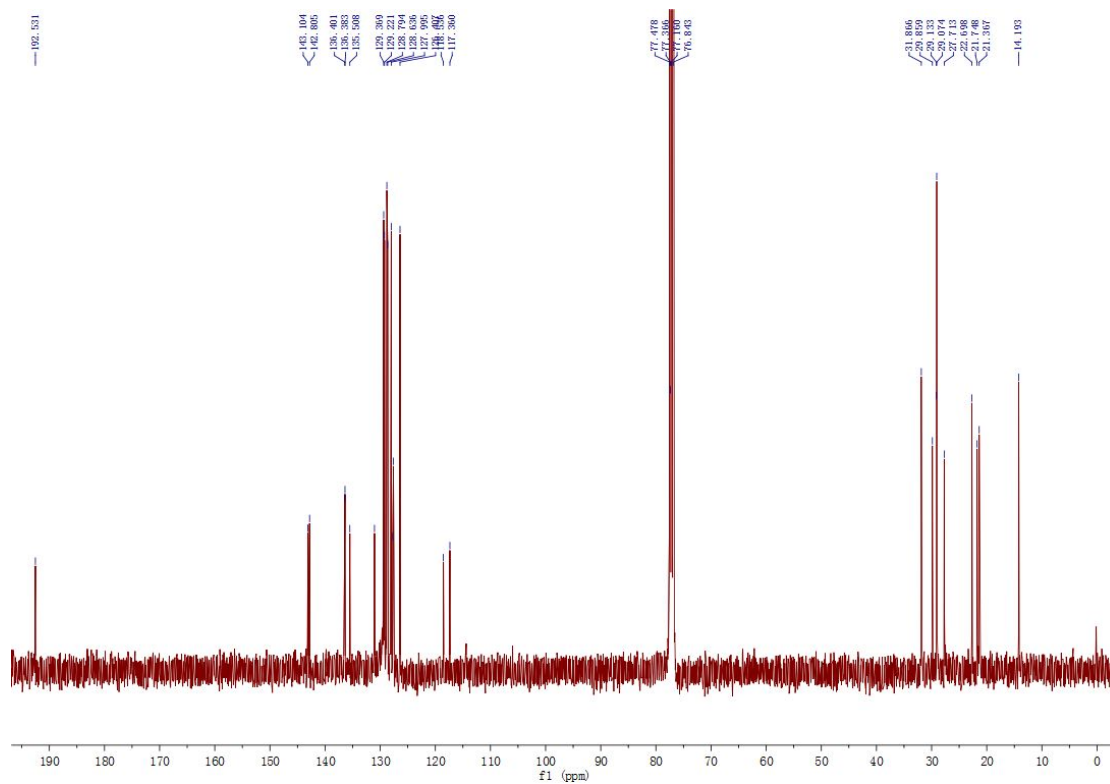
¹H NMR Spectrum for **3m** (CDCl₃, 400 MHz)



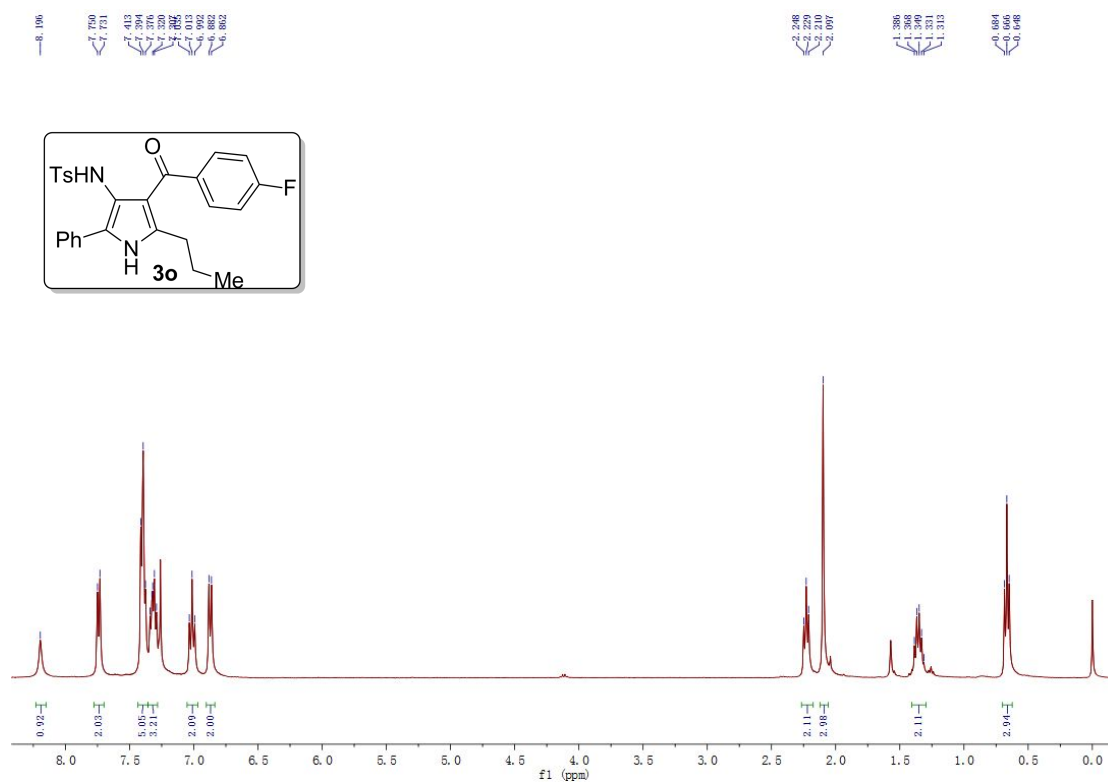
¹³C NMR Spectrum for **3m** (CDCl₃, 100 MHz)



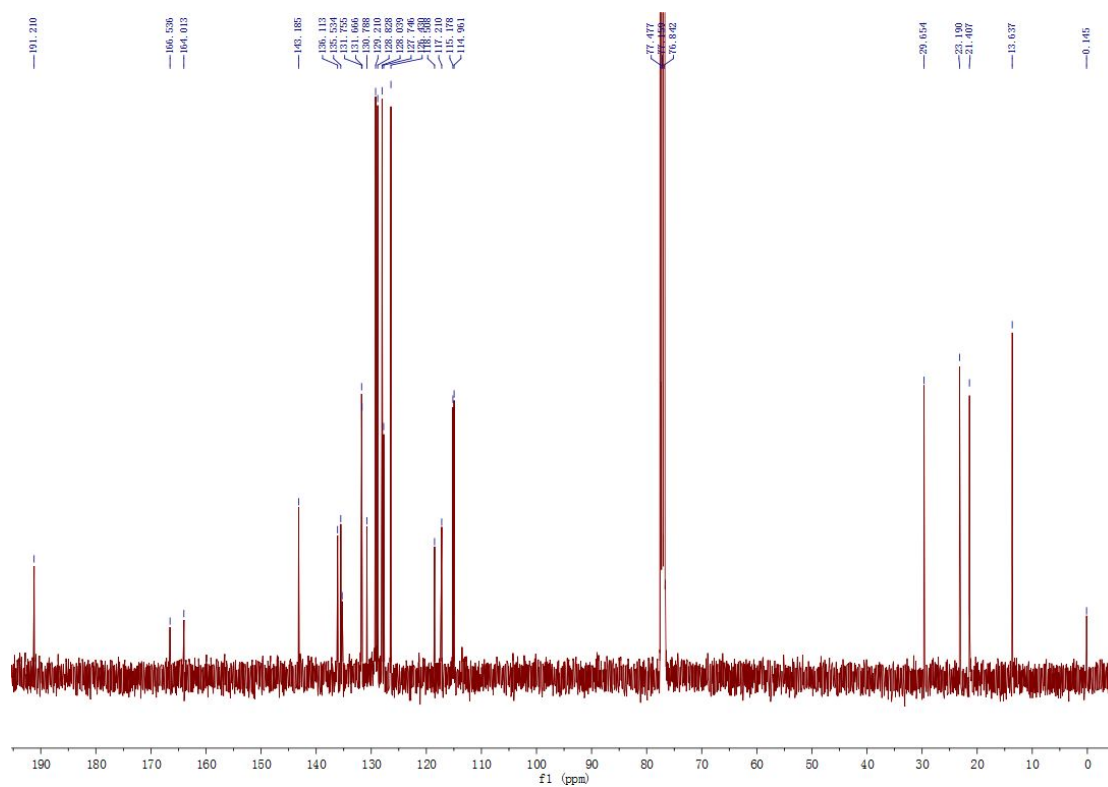
¹H NMR Spectrum for **3n** (CDCl₃, 400 MHz)



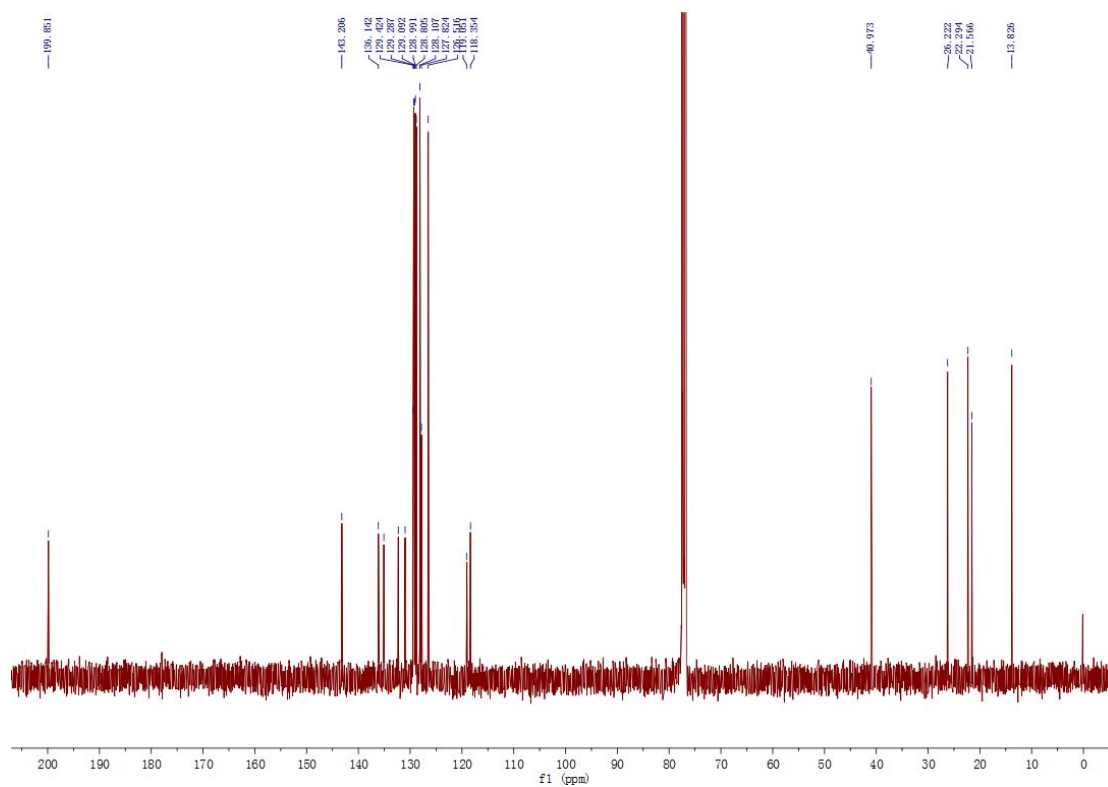
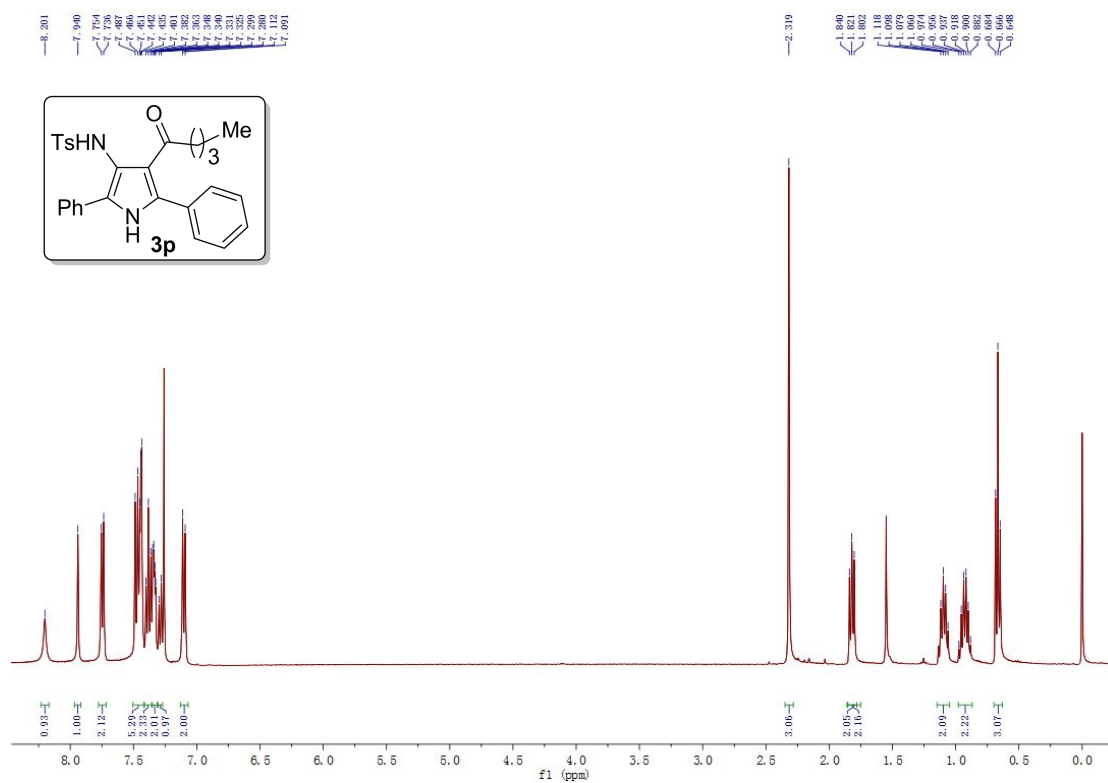
¹³C NMR Spectrum for **3n** (CDCl₃, 100 MHz)

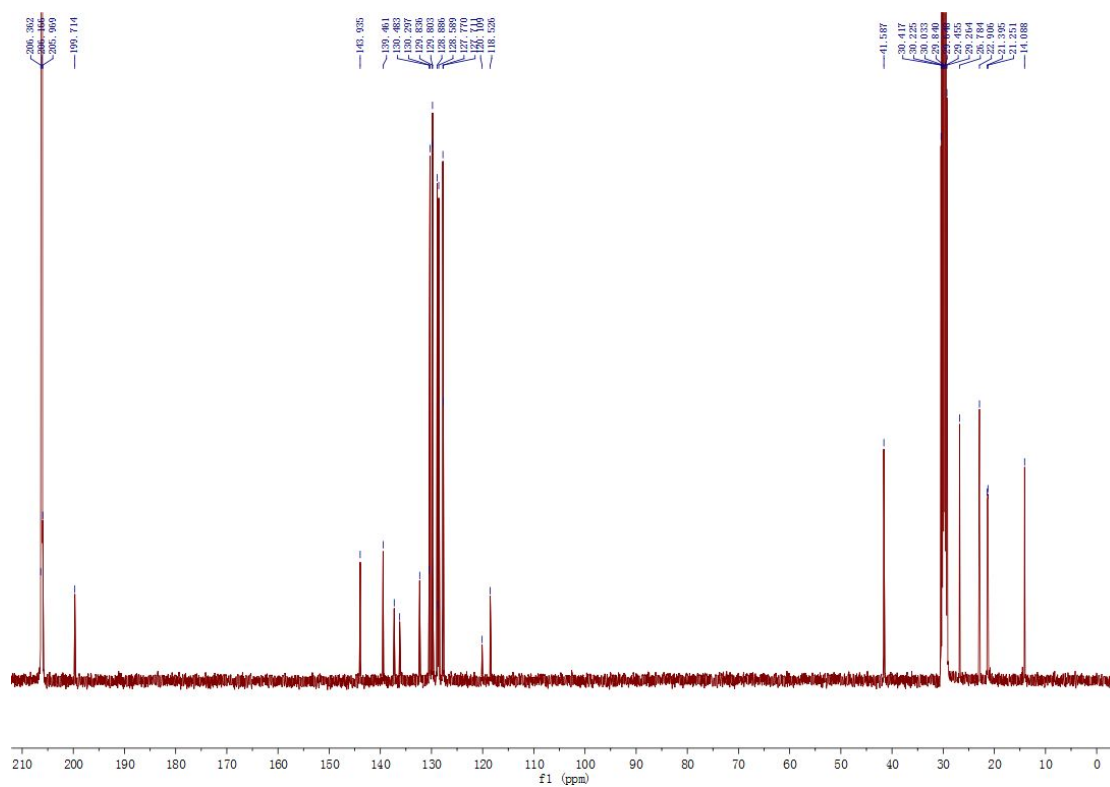
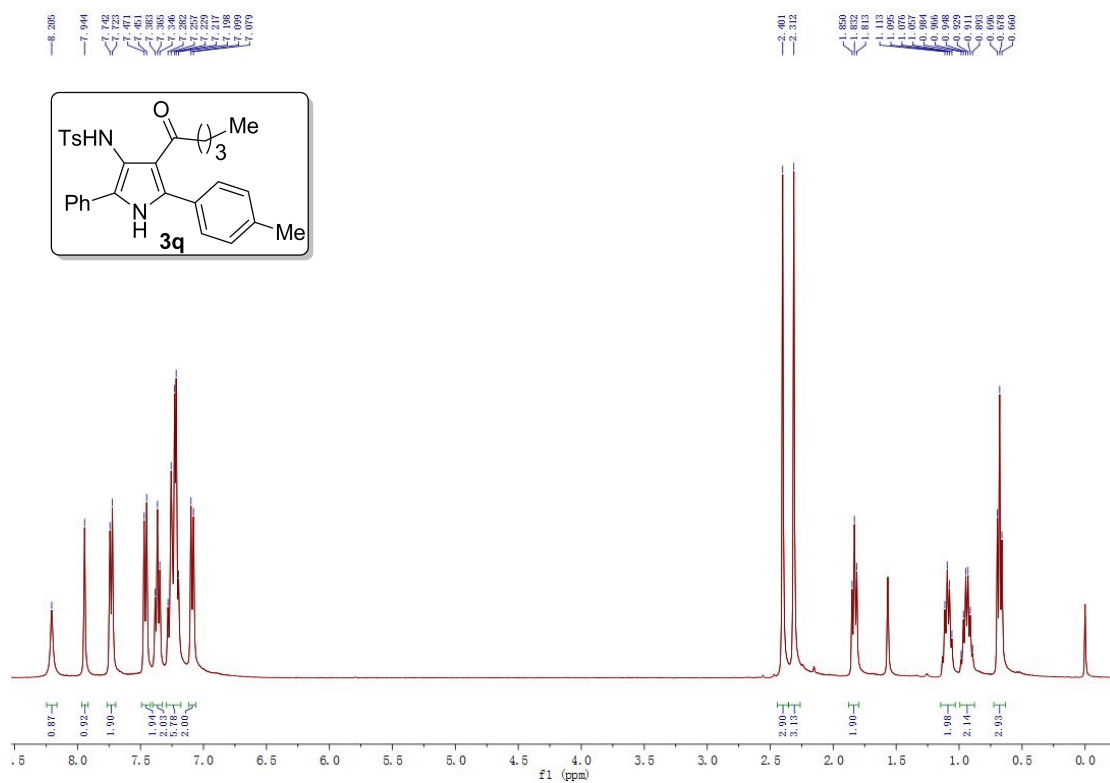


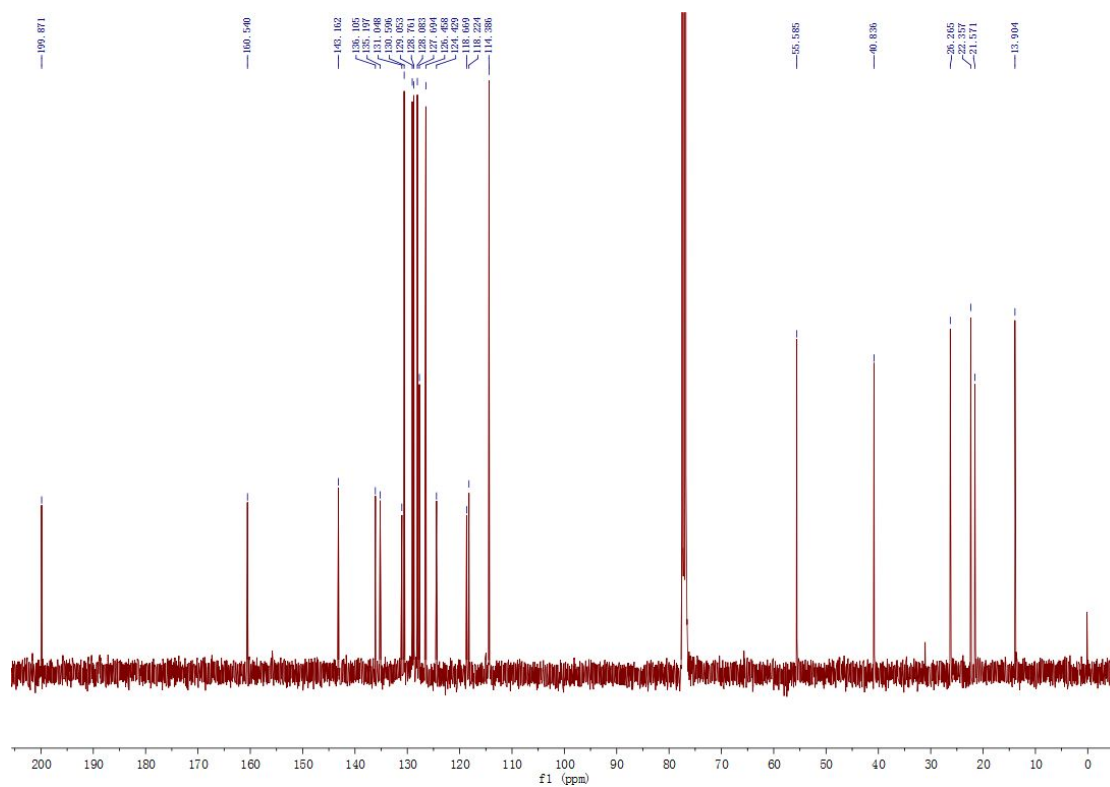
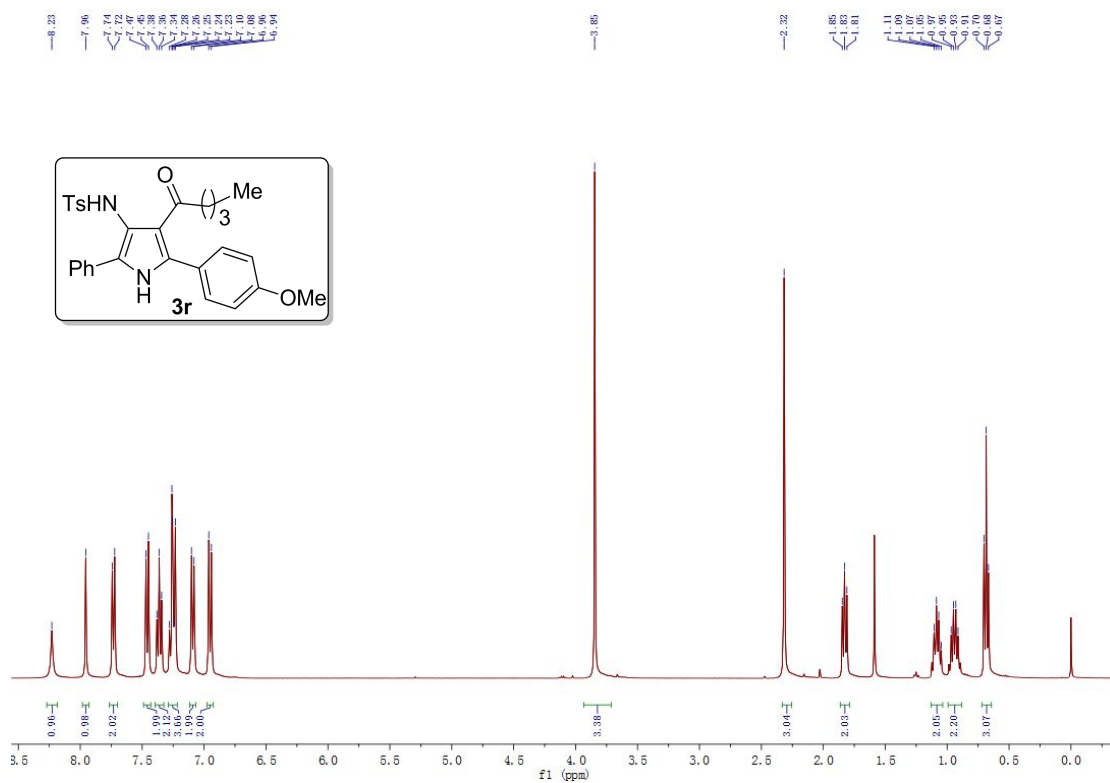
¹H NMR Spectrum for **3o** (CDCl₃, 400 MHz)

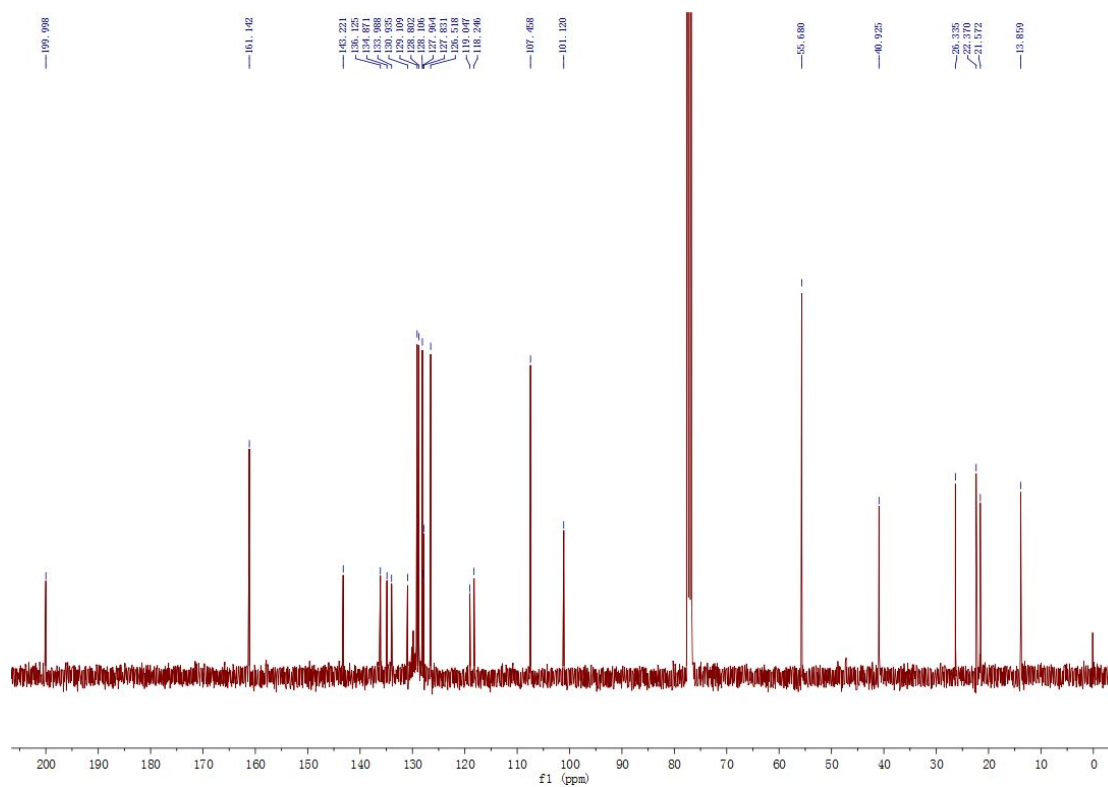
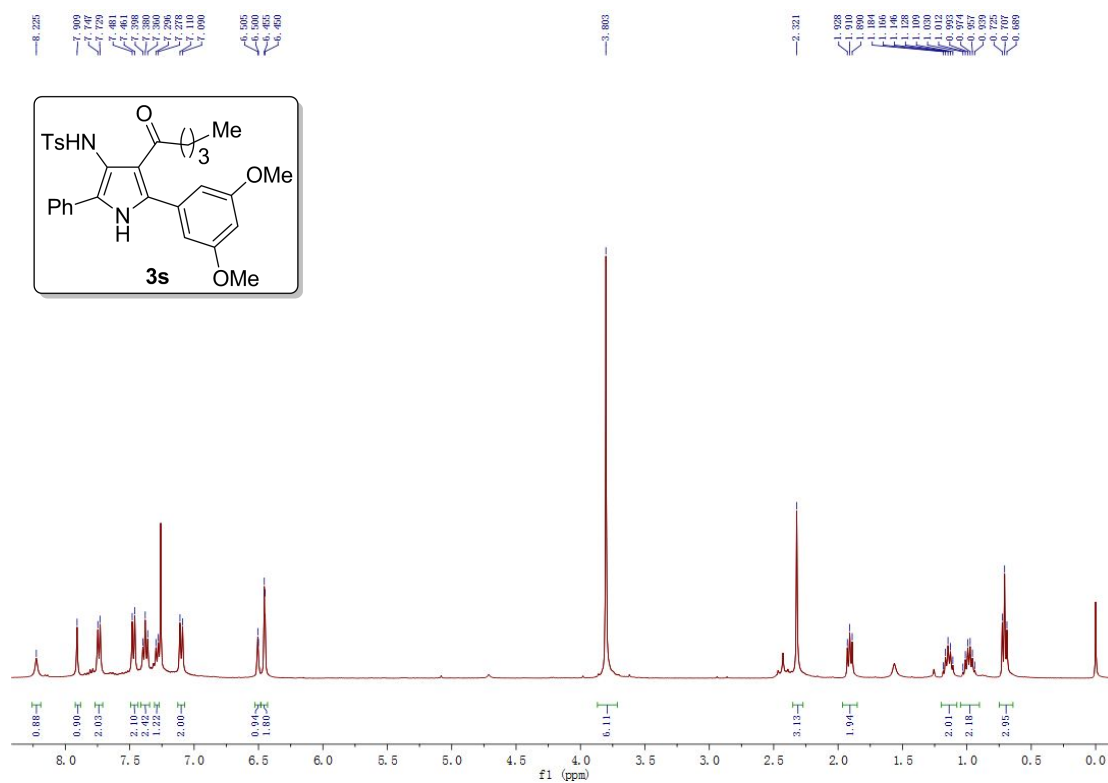


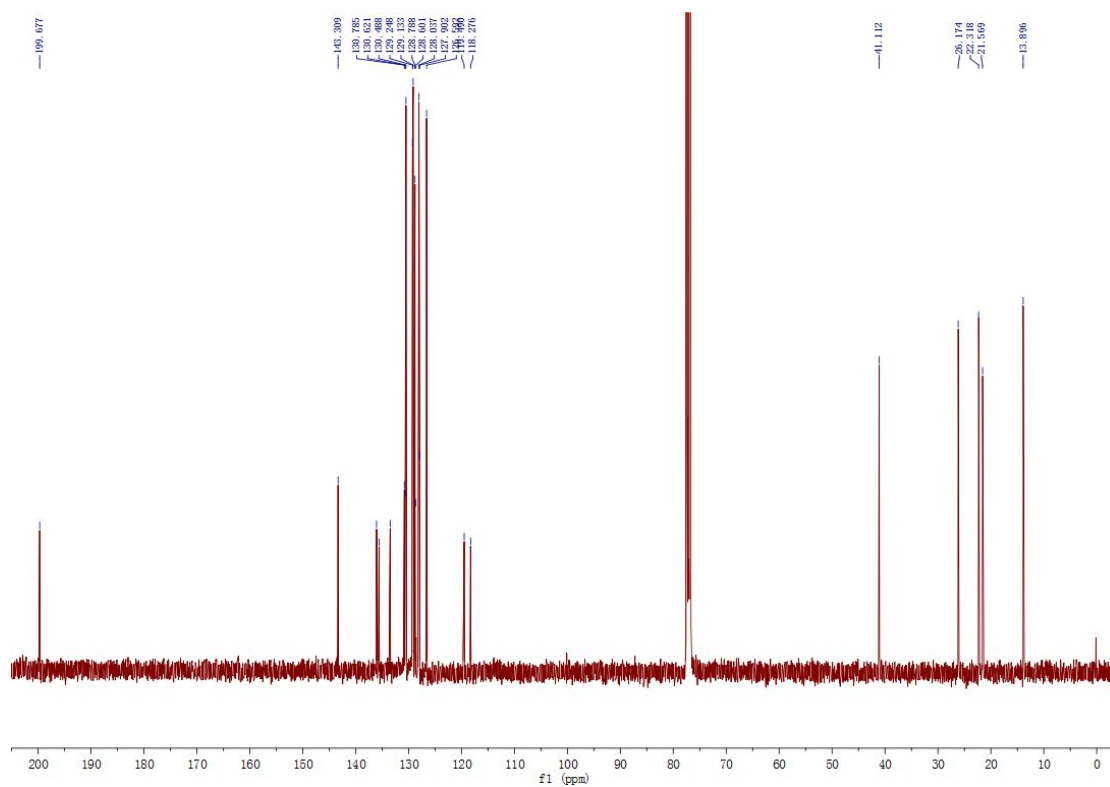
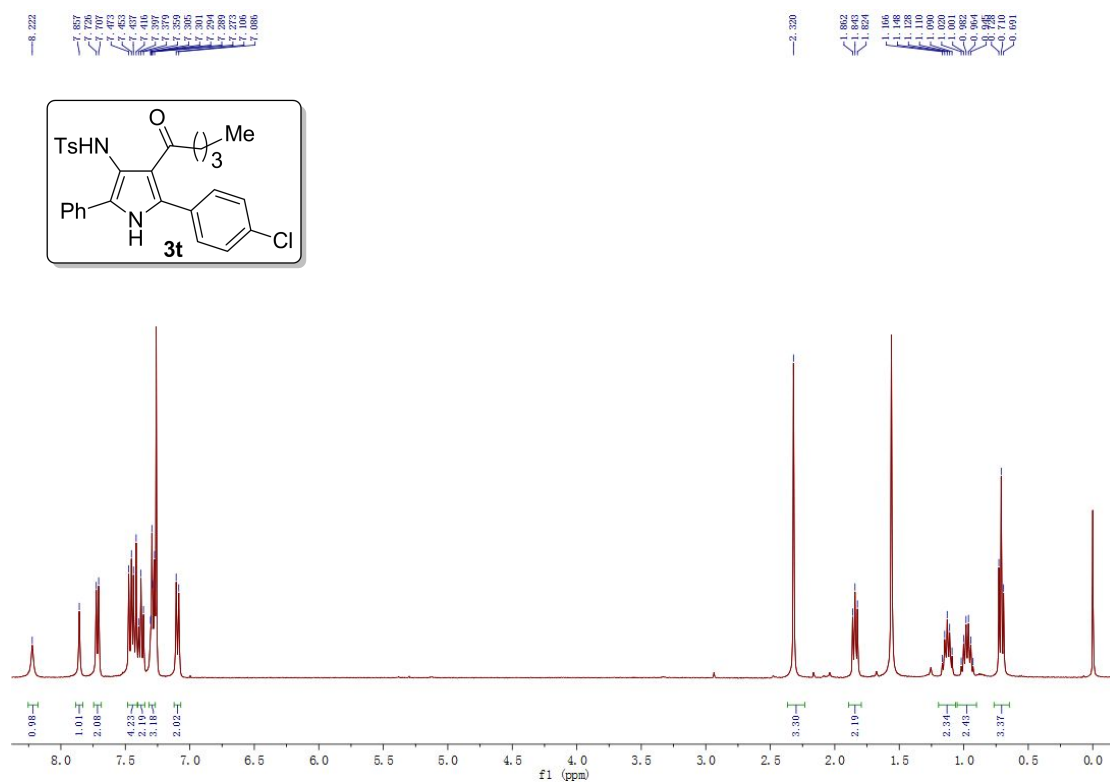
¹³C NMR Spectrum for **3o** (CDCl₃, 100 MHz)

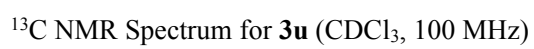
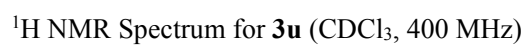


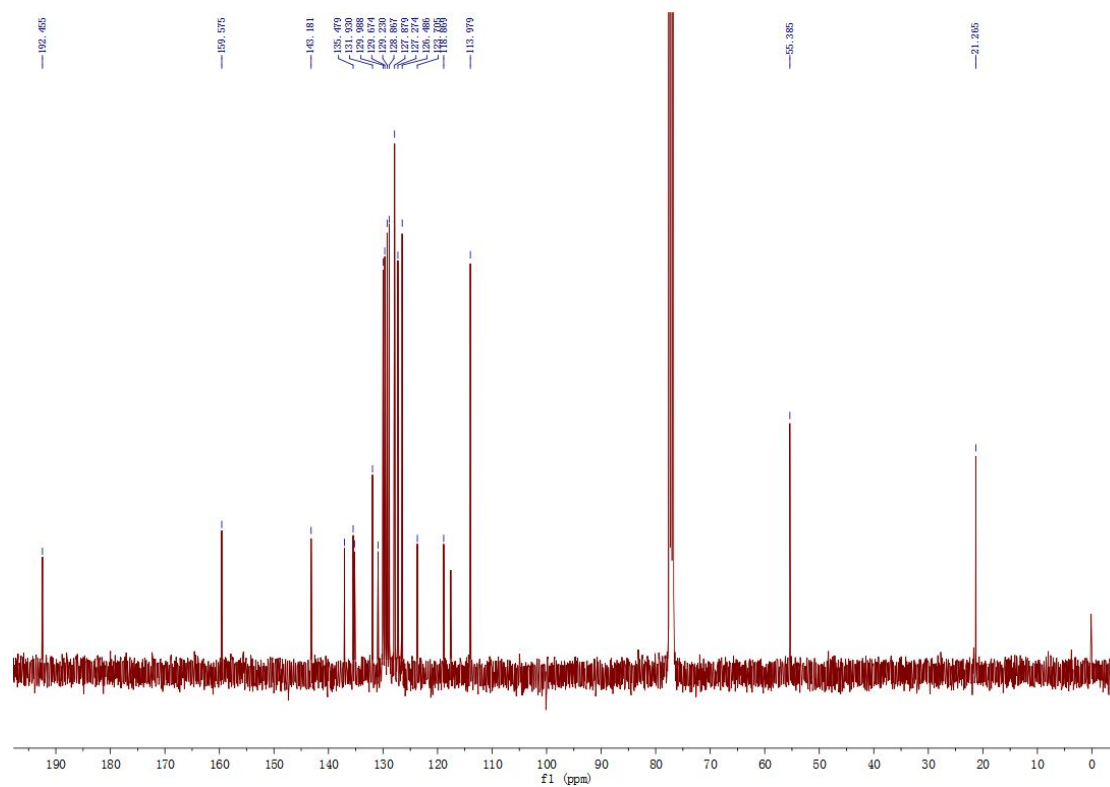
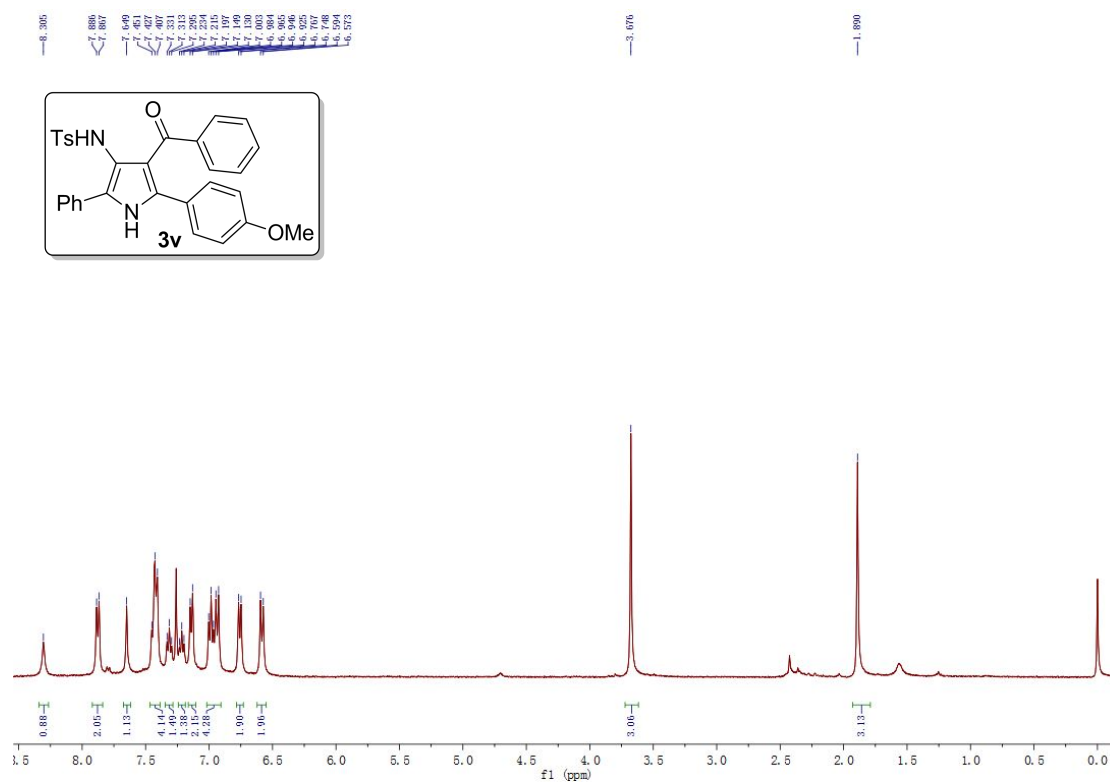


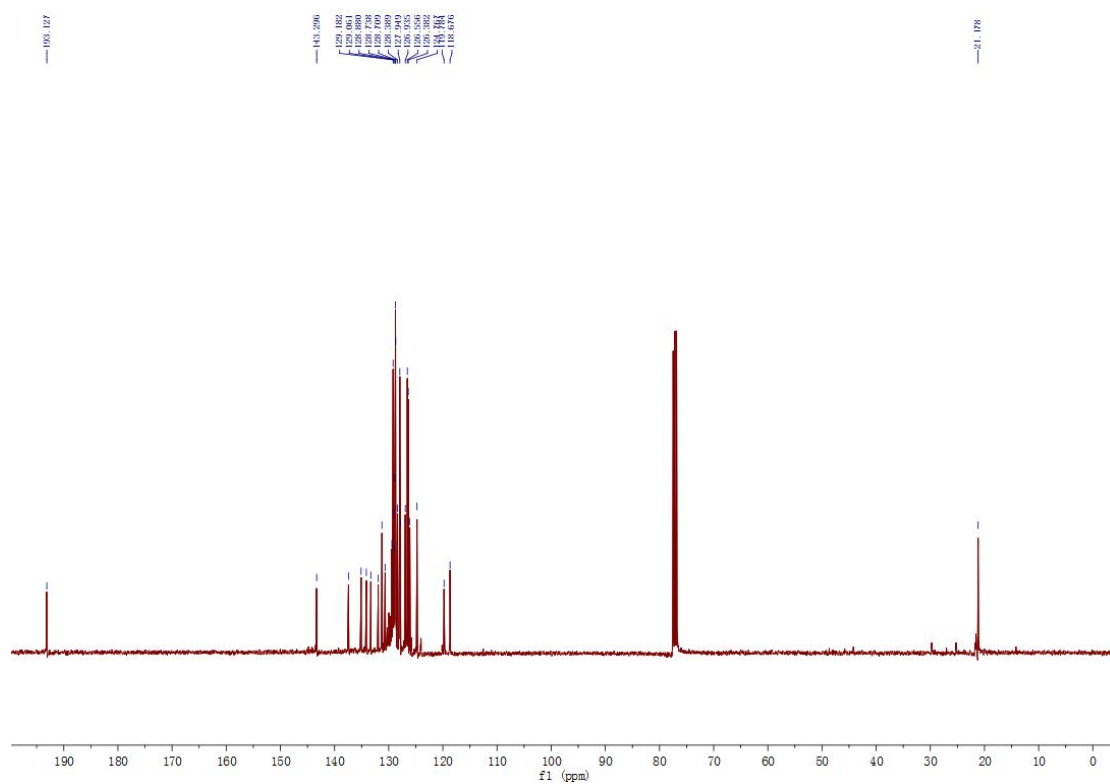
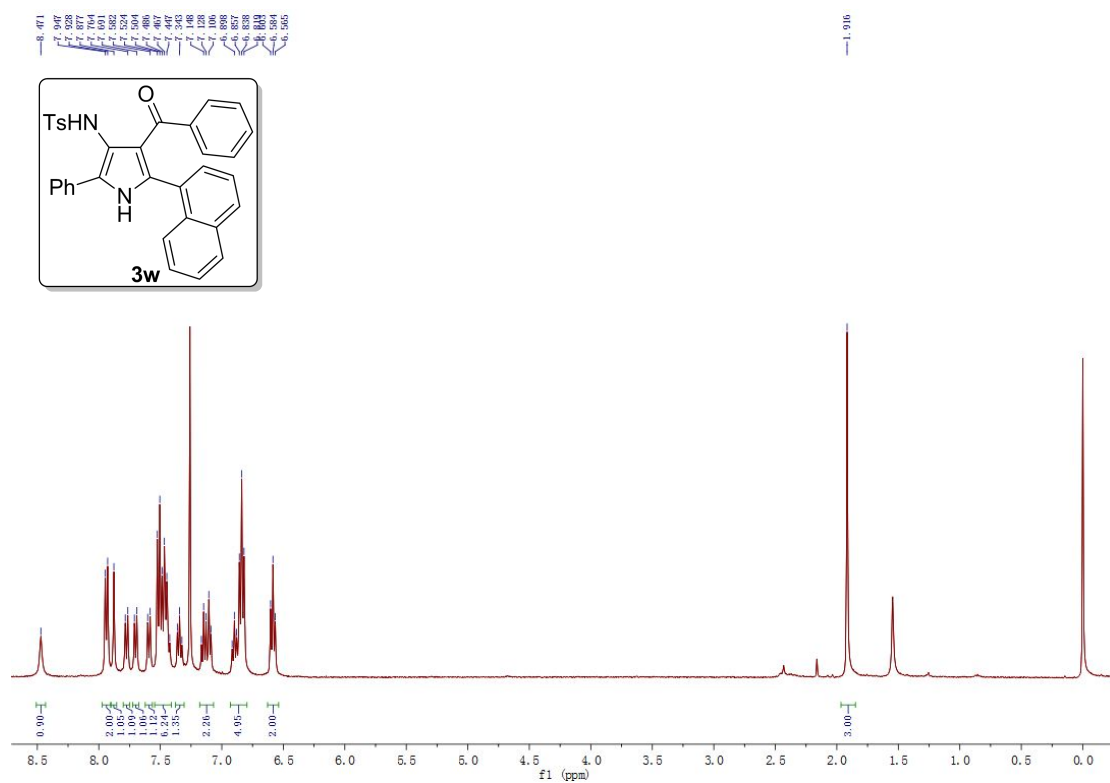


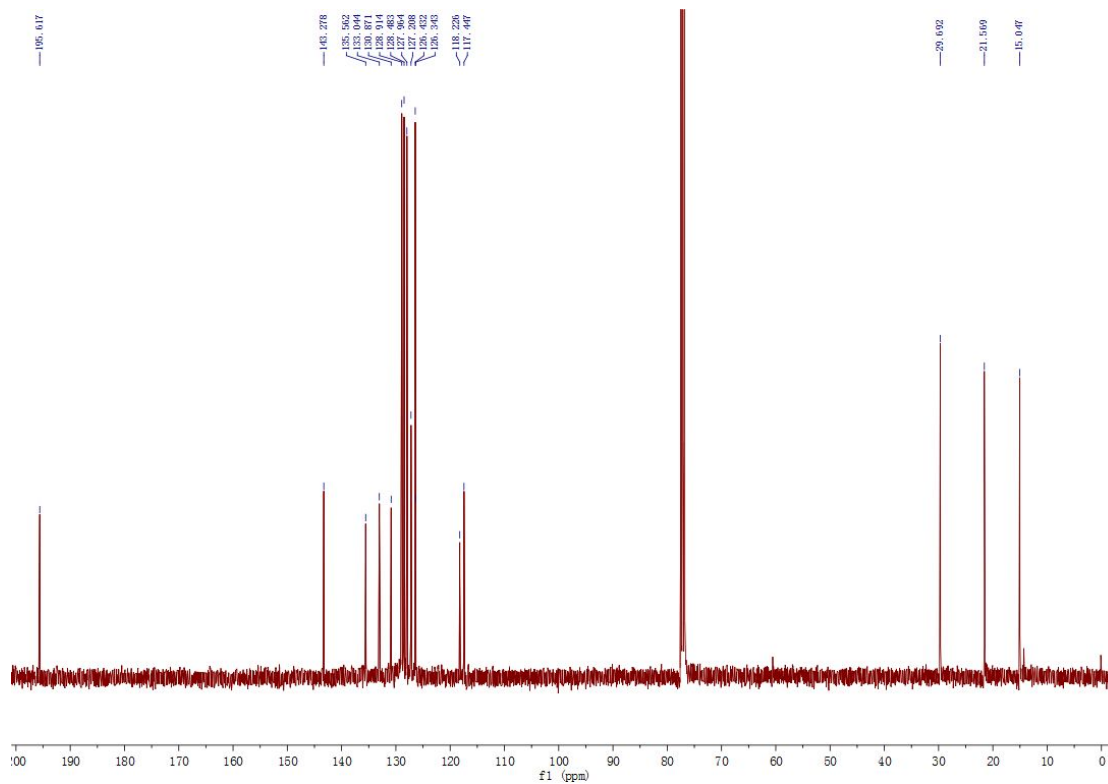
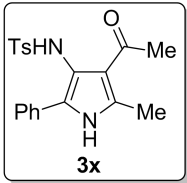


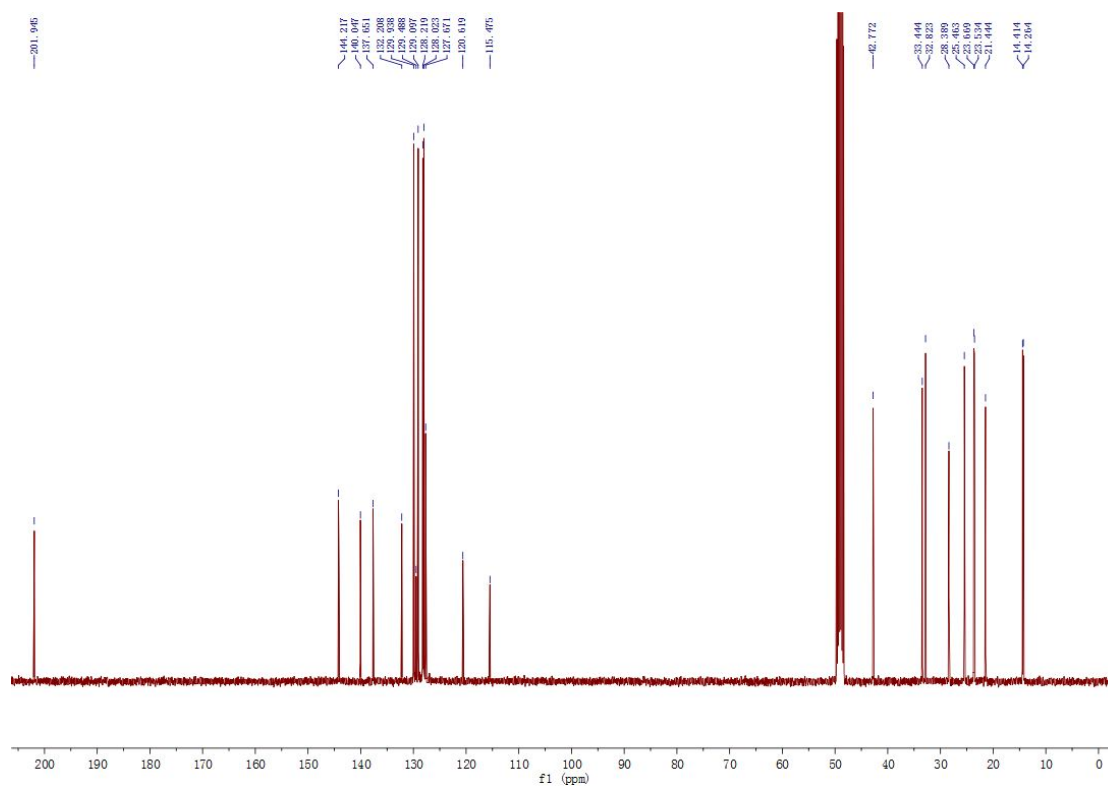
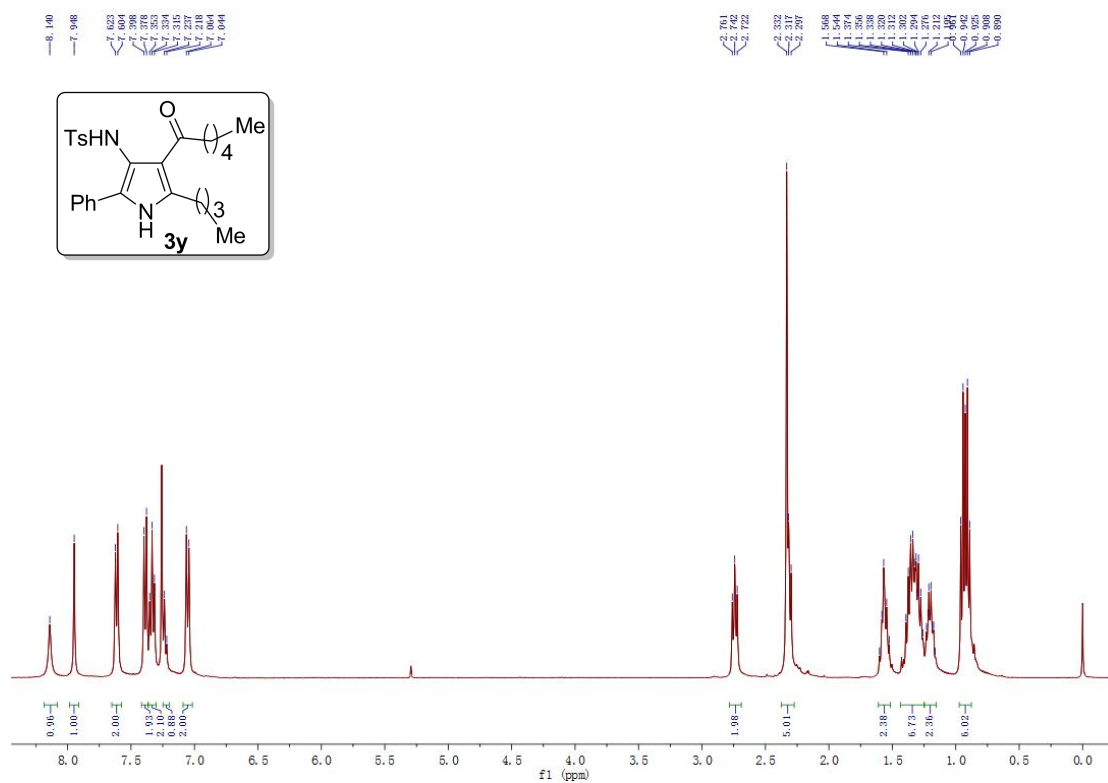


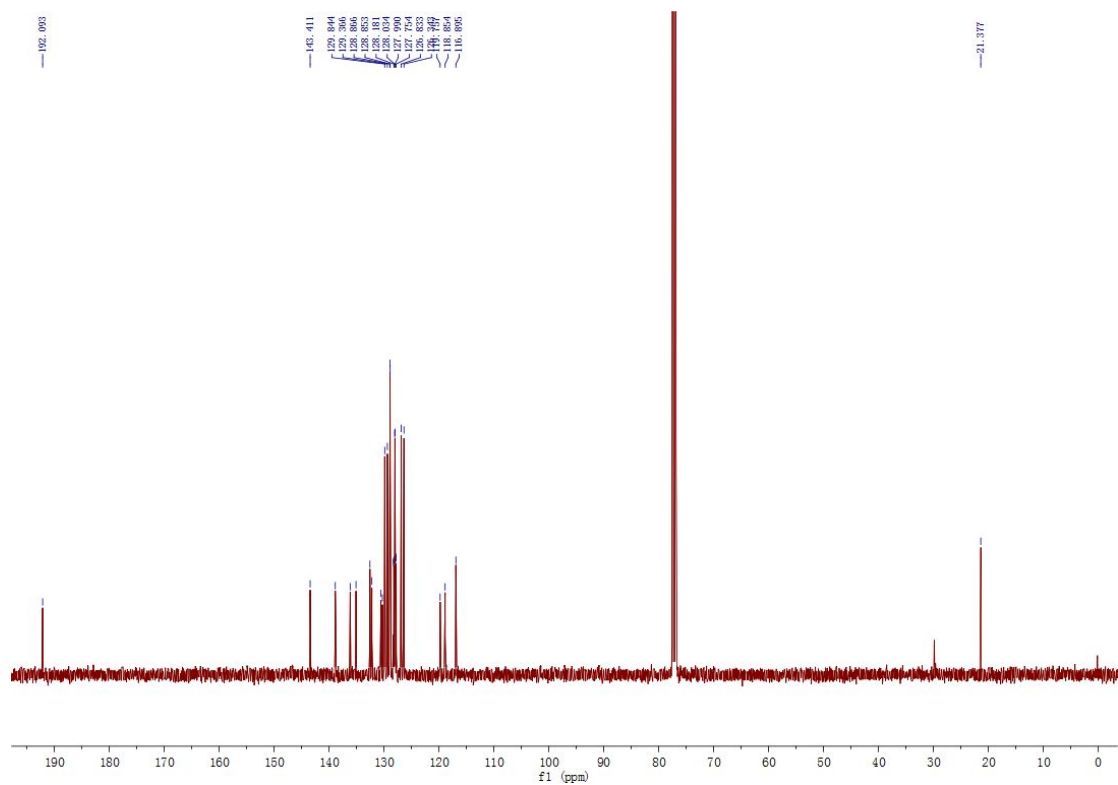
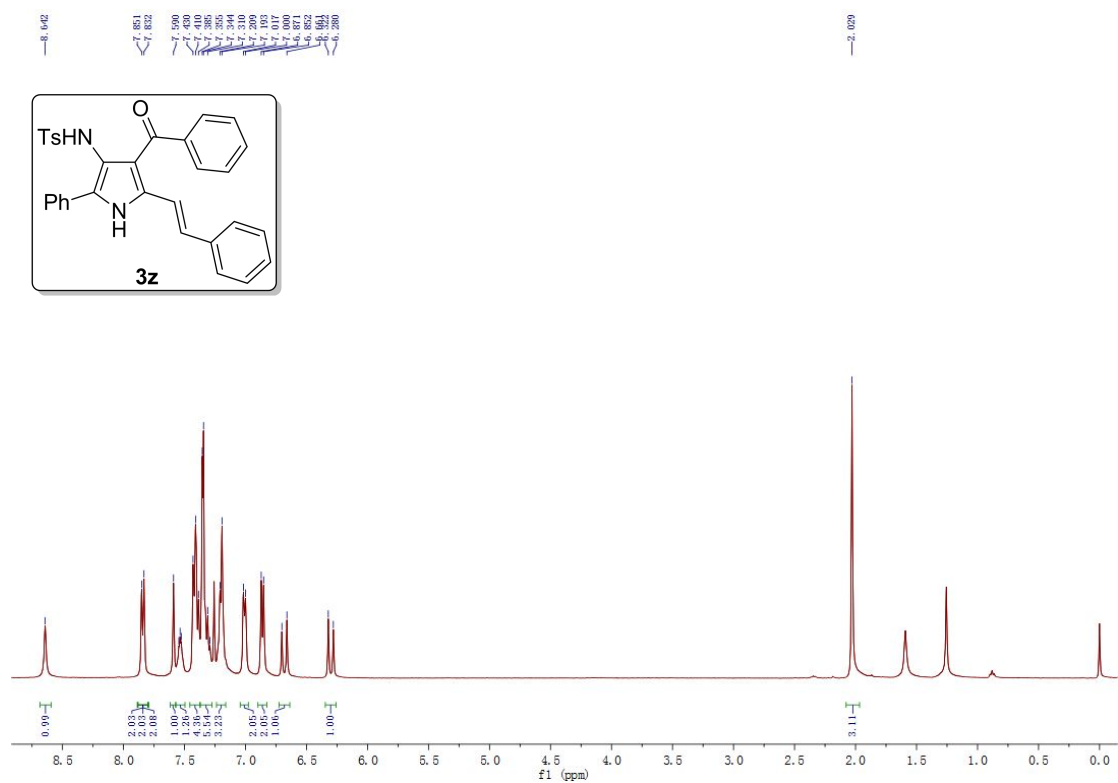




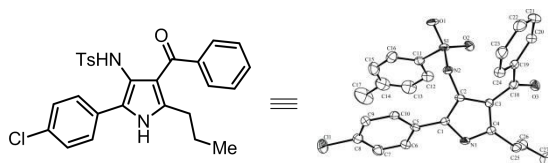








9. X-ray Crystallographic Structure of **3e**



X-ray Crystallographic structure and data of **3e**

Compound	3e
formula	C ₂₇ H ₂₅ Cl N ₂ O ₃ S
FW	535.08
crystal system	monoclinic
space group	<i>P</i> 1 21/ <i>c</i> 1
<i>a</i> /Å	8.5092(7)
<i>b</i> /Å	28.168(3)
<i>c</i> /Å	12.0300(12)
α /deg	90
β /deg	100.513(10)
γ /deg	90
<i>V</i> /Å ³	2835.0(5)
<i>Z</i>	4
<i>D</i> _c /g cm ⁻³	1.254
μ /mm ⁻¹	0.241
<i>R</i> ₁ ^a (<i>I</i> > 2 σ)	0.0842(2649)
w <i>R</i> ₂ ^b (all data)	0.2345(5585)
GOF	1.001