

Synthesis of Thiazolo[2,3-*b*]quinazoline Derivatives via Base-Promoted Cascade Bicyclization of *o*-Alkenylphenyl Isothiocyanates with Propargylamines

Jiankang Miao, Xiaoyan Sang, Yi Wang, Shufeng Deng and Wenyan Hao*

Key Laboratory of Functional Small Organic Molecules, Ministry of Education, and College of Chemistry & Chemical Engineering, Jiangxi Normal University, 99 Ziyang Road, Nanchang, Jiangxi, 330022, P.R. China
Email :wenyanhao@jxnu.edu.cn

Support Information

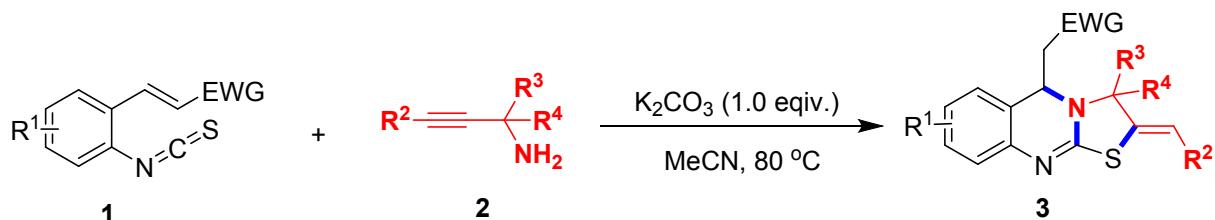
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1. General Information

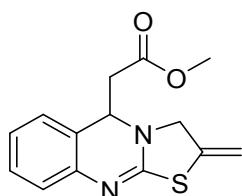
All reagents and metal catalysts were obtained from commercial sources without further purification, and commercially available solvents were purified before use. All reactions were performed in reaction tubes. All new compounds were fully characterized. Silica gel plate GF254 were used for thin layer chromatography (TLC) and silica gel H or 300-400 mesh were used for flash column chromatography. Thin layer chromatography plates were visualized by exposure to ultraviolet light. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. The mass analyzer type used for the HRMS measurements is micro TOF. Yields refer to chromatographically and spectroscopically pure compounds, unless otherwise indicated.

2. Synthesis and Characterization for Compounds 3aa-3sa, 3ab-3an:



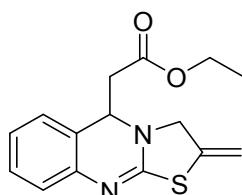
$\text{EWG} = \text{CO}_2\text{R}; \text{CN}, \text{CON}(\text{CH}_3)_2$

A mixture of *o*-alkenylphenyl isothiocyanate **1** (0.20 mmol) and propargylamine **2** (0.3 mmol) K_2CO_3 (0.20 mmol) was added into a tube. Subsequently MeCN (2 mL) was added. Then, the sealed tube was heated at 80 °C for 3 hours. After completion of reaction as indicated by TLC, the mixture was concentrated and directly purified by flash column chromatography (EtOAc/petroleum ether, 1:2) to give the desired product **3**.



methyl 2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3aa)

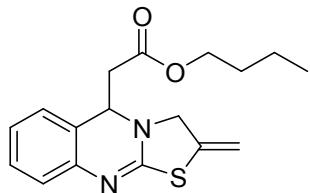
Yellow oil; (52.7 mg, 96%); ^1H NMR (400 MHz, CDCl_3) δ 7.12 (t, $J = 7.4$ Hz, 1H), 6.94 (dd, $J = 8.4, 17.2$ Hz, 2H), 6.87 (d, $J = 7.6$ Hz, 1H), 5.20 (s, 1H), 5.11 (s, 1H), 5.04 (t, $J = 4.8$ Hz, 1H), 4.47 (d, $J = 14.4$ Hz, 1H), 4.23 (d, $J = 14.4$ Hz, 1H), 3.57 (s, 3H), 2.76-2.62 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.9, 160.0, 140.8, 134.3, 128.0, 124.5, 123.6, 122.6, 120.8, 105.1, 55.5, 53.2, 51.1, 39.3; HRMS calcd for $\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2\text{S}^+$ ($\text{M} + \text{H}^+$): 275.0849; Found: 275.0851.



ethyl 2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ba)

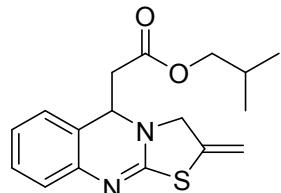
Yellow oil; (51.9 mg, 90%); ^1H NMR (400 MHz, CDCl_3) δ 7.12 (t, $J = 7.4$ Hz, 1H), 6.95 (dd,

J = 8.0, 16.0 Hz, 2H), 6.88 (d, *J* = 7.2 Hz, 1H), 5.19 (d, *J* = 1.2 Hz, 1H), 5.11 (d, *J* = 1.6 Hz, 1H), 5.05 (t, *J* = 5.2 Hz, 1H), 4.50 (d, *J* = 14 Hz, 1H), 4.23 (d, *J* = 14 Hz, 1H), 4.06-3.99 (m, 2H), 2.74-2.62 (m, 2H), 1.11 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.4, 161.0, 141.9, 135.4, 128.9, 125.6, 124.6, 123.7, 121.8, 106.0, 61.1, 56.6, 54.4, 40.6, 14.0; HRMS calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2\text{S}^+$ ($\text{M} + \text{H}^+$): 289.1005; Found: 289.1016.



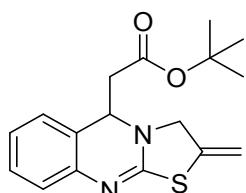
butyl 2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ca)

Yellow oil; (49.4 mg, 78%); ^1H NMR (400 MHz, CDCl_3) δ 7.12 (t, *J* = 7.6 Hz, 1H), 6.96 (dd, *J* = 8.0, 18.8 Hz, 2H), 6.88 (d, *J* = 7.6 Hz, 1H), 5.20 (d, *J* = 2.0 Hz, 1H), 5.12 (d, *J* = 2.0 Hz, 1H), 5.05 (t, *J* = 5.2 Hz, 1H), 4.50 (d, *J* = 14.0 Hz, 1H), 4.24 (d, *J* = 14.0 Hz, 1H), 3.99-3.95 (m, 2H), 2.77-2.63 (m, 2H), 1.49-1.42 (m, 2H), 1.24-1.15 (m, 2H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.6, 161.0, 141.8, 135.4, 128.9, 125.5, 124.6, 123.6, 121.8, 106.0, 65.0, 56.6, 54.4, 40.6, 30.4, 19.0, 13.6; HRMS calcd for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+$ ($\text{M} + \text{H}^+$): 317.1318; Found: 317.1295.



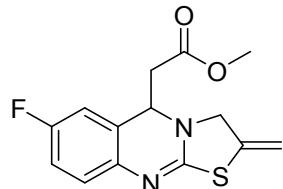
isobutyl 2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3da)

Yellow oil; (58.2 mg, 92%); ^1H NMR (400 MHz, CDCl_3) δ 7.19 (t, *J* = 7.6 Hz, 1H), 7.02 (dd, *J* = 7.6, 18.8 Hz, 2H), 6.96 (d, *J* = 7.6 Hz, 1H), 5.27 (d, *J* = 2.0 Hz, 1H), 5.19 (d, *J* = 2.0 Hz, 1H), 5.13 (t, *J* = 5.6 Hz, 1H), 4.58 (td, *J* = 2.0, 14.4 Hz, 1H), 4.32 (td, *J* = 2.0, 14.4 Hz, 1H), 3.82 (d, *J* = 8.8 Hz, 2H), 2.86-2.72 (m, 2H), 1.89-1.79 (m, 1H), 0.84 (dd, *J* = 2.8, 6.4 Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.6, 161.0, 141.8, 135.4, 128.9, 125.5, 124.6, 123.7, 121.9, 106.0, 71.3, 56.6, 54.4, 40.5, 27.5, 19.0; HRMS calcd for $\text{C}_{17}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+$ ($\text{M} + \text{H}^+$): 317.1318; Found: 317.1324.



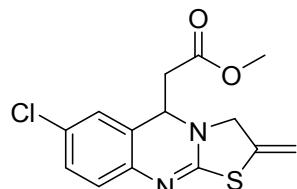
tert-butyl 2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ea)

Pale green oil; (60.8 mg, 96%); ¹H NMR (400 MHz, CDCl₃) δ 7.11 (t, *J* = 7.4 Hz, 1H), 6.97-6.89 (m, 3H), 5.19 (d, *J* = 2.0 Hz, 1H), 5.11 (d, *J* = 2.0 Hz, 1H), 5.02 (t, *J* = 5.2 Hz, 1H), 4.54 (d, *J* = 14.4 Hz, 1H), 4.22 (d, *J* = 14.4 Hz, 1H), 2.63 (d, *J* = 5.2 Hz, 2H), 1.29 (s, 9H); ¹³C NMR (100 MHz, CDCl₃) δ 168.5, 159.9, 140.8, 134.4, 127.8, 124.6, 123.4, 122.6, 120.7, 104.8, 80.5, 55.6, 53.6, 40.8, 26.8; HRMS calcd for C₁₇H₂₁N₂O₂S⁺ (M + H⁺): 317.1318; Found: 317.1314.



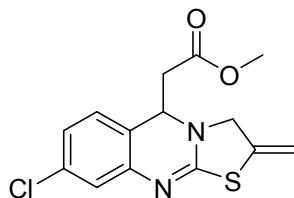
Methyl 2-(7-fluoro-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3fa)

Yellow oil; (57.3 mg, 98%); ¹H NMR (400 MHz, CDCl₃) δ 6.95-6.89 (m, 1H), 6.82 (dt, *J* = 2.8, 8.4 Hz, 1H), 6.61 (dd, *J* = 2.8, 8.8 Hz, 1H), 5.21 (d, *J* = 2.0 Hz, 1H), 5.12 (d, *J* = 2.0 Hz, 1H), 5.01 (t, *J* = 5.2 Hz, 1H), 4.46 (d, *J* = 14 Hz, 1H), 4.23 (d, *J* = 14 Hz, 1H), 3.58 (s, 3H), 2.76-2.63 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 170.6, 160.5, 159.6 (d, ¹J_{CF} = 241 Hz), 138.2, 135.2, 125.0 (d, ³J_{CF} = 8 Hz), 123.1 (d, ³J_{CF} = 8 Hz), 115.7 (d, ²J_{CF} = 22 Hz), 112.1 (d, ²J_{CF} = 23 Hz), 106.2, 56.4, 54.1, 52.1, 39.9; HRMS calcd for C₁₄H₁₄FN₂O₂S⁺ (M + H⁺): 293.0755; Found: 293.0750.



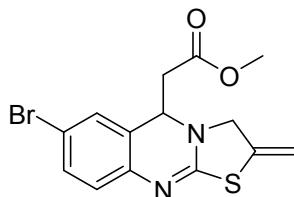
methyl 2-(7-chloro-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ga)

Pale yellow solid; (56.2 mg, 91%); ¹H NMR (400 MHz, CDCl₃) δ 7.08 (dd, *J* = 2.4, 8.4 Hz, 1H), 6.91-6.86 (m, 2H), 5.22 (d, *J* = 1.6 Hz, 1H), 5.13 (d, *J* = 2.0 Hz, 1H), 5.01 (t, *J* = 5.2 Hz, 1H), 4.48 (td, *J* = 2.4, 14 Hz, 1H), 4.25 (td, *J* = 2.4, 14 Hz, 1H), 3.60 (s, 3H), 2.76-2.63 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 170.6, 161.4, 140.7, 135.1, 129.2, 129.0, 125.4, 125.0, 123.3, 106.4, 56.5, 53.9, 52.2, 40.2; HRMS calcd for C₁₄H₁₄ClN₂O₂S⁺ (M + H⁺): 309.0459; Found: 309.0463.



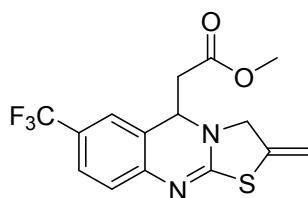
methyl 2-(8-chloro-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ha)

Yellow oil; (58.7 mg, 95%); ¹H NMR (400 MHz, CDCl₃) δ 7.02 (d, *J* = 2.0 Hz, 1H), 6.97 (dd, *J* = 2.0, 8.0 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 5.30 (q, *J* = 2.0 Hz, 1H), 5.21 (q, *J* = 2.4 Hz, 1H), 5.09 (t, *J* = 5.2 Hz, 1H), 4.56 (td, *J* = 2.4, 14 Hz, 1H), 4.33 (td, *J* = 2.4, 14 Hz, 1H), 3.66 (s, 3H), 2.82-2.69 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 170.6, 162.2, 143.3, 135.0, 134.3, 126.6, 124.3, 123.5, 120.3, 106.5, 56.5, 53.9, 52.2, 40.1; HRMS calcd for C₁₄H₁₄ClN₂O₂S⁺ (M + H⁺): 309.0459; Found: 309.0456.



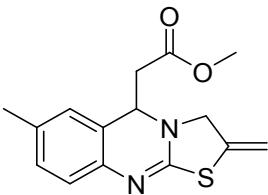
methyl 2-(7-bromo-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ia)

Yellow oil; (64.3 mg, 91%); ¹H NMR (400 MHz, CDCl₃) δ 7.29 (dd, *J* = 2.0, 8.4 Hz, 1H), 7.08 (s, 1H), 6.91 (dd, *J* = 2.0, 8.4 Hz, 1H), 5.29 (t, *J* = 1.6 Hz, 1H), 5.21 (t, *J* = 2.0 Hz, 1H), 5.08 (t, *J* = 5.2 Hz, 1H), 4.55 (dd, *J* = 1.6, 14.0 Hz, 1H), 4.32 (dd, *J* = 1.6, 14.0 Hz, 1H), 3.67 (s, 3H), 2.83-2.70 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 170.6, 161.5, 141.2, 135.1, 132.0, 128.3, 125.4, 123.7, 116.7, 106.4, 56.5, 53.8, 52.2, 40.3; HRMS calcd for C₁₄H₁₄BrN₂O₂S⁺ (M + H⁺): 352.9954; Found: 352.9953;



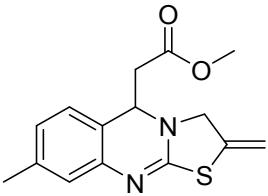
methyl 2-(2-methylene-7-(trifluoromethyl)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ja)

White solid; (53.4 mg, 78%); ¹H NMR (400 MHz, CDCl₃) δ 7.45 (d, *J* = 8.4 Hz, 1H), 7.20 (s, 1H), 7.11 (d, *J* = 8.4 Hz, 1H), 5.32 (q, *J* = 2.0 Hz, 1H), 5.23 (q, *J* = 2.0 Hz, 1H), 5.17 (t, *J* = 5.6 Hz, 1H), 4.61 (td, *J* = 2.4, 14.4 Hz, 1H), 4.38 (td, *J* = 2.4, 14.4 Hz, 1H), 3.66 (s, 3H), 2.88-2.72 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 170.4, 163.2, 145.0, 134.7, 126.2 (q, *J*_{CF₃} = 4 Hz), 125.9, 123.8, 122.8, 122.1, 106.7, 56.6, 54.1, 52.2, 40.2; HRMS calcd for C₁₅H₁₄F₃N₂O₂S⁺ (M + H⁺): 343.0723; Found: 343.0710.



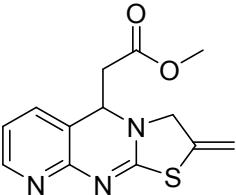
methyl 2-(7-methyl-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ka)

Yellow oil; (55.9 mg, 97%); ^1H NMR (400 MHz, CDCl_3) δ 7.01 (d, $J = 8.0$ Hz, 1H), 6.95 (d, $J = 8.0$ Hz, 1H), 6.76 (s, 1H), 5.27 (d, $J = 2.0$ Hz, 1H), 5.18 (d, $J = 2.0$ Hz, 1H), 5.08 (t, $J = 5.6$ Hz, 1H), 4.54 (td, $J = 2.0, 14.4$ Hz, 1H), 4.30 (td, $J = 2.0, 14.4$ Hz, 1H), 3.66 (s, 3H), 2.84-2.70 (m, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.1, 160.2, 139.5, 135.6, 134.3, 129.7, 125.9, 123.5, 121.7, 105.9, 56.6, 54.4, 52.1, 40.5, 21.0; HRMS calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2\text{S}^+$ ($M + \text{H}^+$): 289.1005; Found: 289.1004.



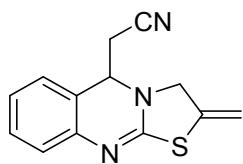
methyl 2-(8-methyl-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3la)

Yellow oil; (54.8 mg, 95%); ^1H NMR (400 MHz, CDCl_3) δ 6.86 (d, $J = 13.6$ Hz, 3H), 5.27 (d, $J = 1.6$ Hz, 1H), 5.19 (d, $J = 2.0$ Hz, 1H), 5.10 (t, $J = 5.4$ Hz, 1H), 4.55 (d, $J = 14$ Hz, 1H), 4.31 (d, $J = 14.4$ Hz, 1H), 3.66 (s, 3H), 2.83-2.69 (m, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.0, 160.9, 141.6, 138.8, 135.5, 125.4, 125.2, 124.2, 119.0, 105.9, 56.6, 54.2, 52.1, 40.4, 21.1; HRMS calcd for $\text{C}_{15}\text{H}_{17}\text{N}_2\text{O}_2\text{S}^+$ ($M + \text{H}^+$): 289.1005; Found: 289.1006.



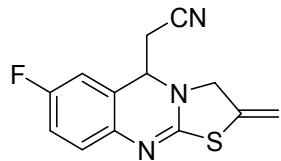
methyl 2-(2-methylene-2,3-dihydro-5H-pyrido[2,3-d]thiazolo[3,2-a]pyrimidin-5-yl)acetate(3ma)

Yellow solid; (41.9 mg, 76%); ^1H NMR (400 MHz, CDCl_3) δ 8.23 (dd, $J = 1.2, 4.8$ Hz, 1H), 7.23 (d, $J = 8.4$ Hz, 1H), 6.85 (q, $J = 4.8$ Hz, 1H), 5.23 (d, $J = 2.0$ Hz, 1H), 5.14 (d, $J = 2.0$ Hz, 1H), 5.11 (t, $J = 5.6$ Hz, 1H), 4.53 (td, $J = 2.0, 14.4$ Hz, 1H), 4.30 (td, $J = 2.0, 14.4$ Hz, 1H), 3.59 (s, 3H), 2.80-2.66 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.5, 165.4, 154.2, 149.3, 135.0, 134.2, 119.6, 116.6, 106.6, 56.5, 54.3, 52.2, 40.1; HRMS calcd for $\text{C}_{13}\text{H}_{14}\text{N}_3\text{O}_2\text{S}^+$ ($M + \text{H}^+$): 276.0801; Found: 276.0809.



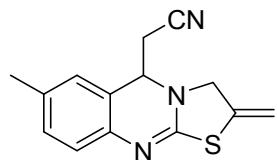
2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetonitrile(3na)

White solid; (36.2 mg, 75%); ^1H NMR (400 MHz, CDCl_3) δ 7.20 (t, $J = 7.2$ Hz, 1H), 7.04-6.97 (m, 3H), 5.26 (s, 1H), 5.17 (s, 1H), 4.94 (s, 1H), 4.65 (d, $J = 14.0$ Hz, 1H), 4.31 (d, $J = 14$ Hz, 1H), 2.77-2.64 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.6, 141.7, 134.4, 129.9, 125.7, 125.1, 124.2, 119.7, 116.8, 106.9, 56.6, 54.4, 24.2; HRMS calcd for $\text{C}_{13}\text{H}_{12}\text{N}_3\text{S}^+$ ($M + \text{H}^+$): 242.0746; Found: 242.0769.



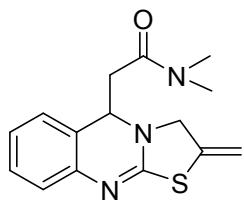
2-(7-fluoro-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetonitrile(3oa)

White solid; (78.2 mg, 95%); ^1H NMR (400 MHz, CDCl_3) δ 7.08 (dd, $J = 5.2, 8.4$ Hz, 1H), 6.99 (dt, $J = 2.4, 8.4$ Hz, 1H), 6.79 (dd, $J = 2.4, 8.4$ Hz, 1H), 5.35 (d, $J = 2.0$ Hz, 1H), 5.26 (d, $J = 2.0$ Hz, 1H), 5.02 (t, $J = 5.2$ Hz, 1H), 4.73 (d, $J = 13.6$ Hz, 1H), 4.40 (d, $J = 14.0$ Hz, 1H), 2.87-2.73 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.1, 159.8 (d, ${}^1J_{\text{CF}} = 243$ Hz), 138.2, 134.3, 125.8 (d, ${}^3J_{\text{CF}} = 8$ Hz), 120.7 (d, ${}^3J_{\text{CF}} = 8$ Hz), 116.8 (d, ${}^2J_{\text{CF}} = 23$ Hz), 116.5, 112.3 (d, ${}^2J_{\text{CF}} = 24$ Hz), 107.0, 56.5, 54.3, 24.0; HRMS calcd for $\text{C}_{13}\text{H}_{11}\text{FN}_3\text{S}^+$ ($M + \text{H}^+$): 260.0652; Found: 260.0654.



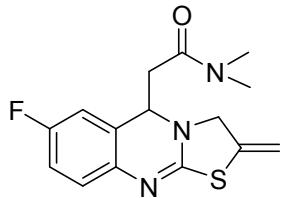
2-(7-methyl-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetonitrile(3pa)

White solid; (49.5 mg, 97%); ^1H NMR (400 MHz, CDCl_3) δ 7.01 (d, $J = 7.6$ Hz, 1H), 6.93 (d, $J = 8.0$ Hz, 1H), 6.78 (s, 1H), 5.26 (s, 1H), 5.17 (s, 1H), 4.91 (t, $J = 4.8$ Hz, 1H), 4.66 (d, $J = 14.0$ Hz, 1H), 4.31 (d, $J = 13.6$ Hz, 1H), 2.77-2.63 (m, 2H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.7, 139.3, 134.9, 134.7, 130.6, 126.0, 124.1, 119.5, 116.9, 106.7, 56.6, 54.6, 24.2, 21.0; HRMS calcd for $\text{C}_{14}\text{H}_{14}\text{N}_3\text{S}^+$ ($M + \text{H}^+$): 256.0903; Found: 256.0890.



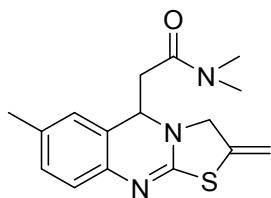
N,N-dimethyl-2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetamide(3qa)

White oil; (50.6 mg, 88%); ¹H NMR (400 MHz, CDCl₃) δ 7.15-7.11 (m, 1H), 6.99-6.88 (m, 3H), 5.20 (d, *J* = 2.0 Hz, 1H), 5.17 (t, *J* = 6.0 Hz, 1H), 5.11 (d, *J* = 2.0 Hz, 1H), 4.55 (td, *J* = 2.0, 14.8 Hz, 1H), 4.33 (td, *J* = 2.0, 14.8 Hz, 1H), 2.84 (s, 3H), 2.77 (dd, *J* = 6.0, 15.2 Hz, 1H), 2.63 (s, 3H), 2.58 (dd, *J* = 6.0, 15.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 169.6, 161.3, 142.1, 135.9, 128.8, 125.6, 124.4, 123.3, 122.8, 105.9, 56.9, 54.3, 39.2, 37.3, 35.6; HRMS calcd for C₁₅H₁₈N₃OS⁺ (M + H⁺): 288.1165; Found: 288.1202.



2-(7-fluoro-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)-N,N-dimethylacetamide(3ra)

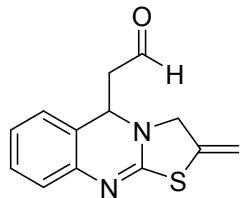
White oil; (60.5 mg, 99%); ¹H NMR (400 MHz, CDCl₃) δ 7.13 (dd, *J* = 5.6, 8.8 Hz, 1H), 6.89 (dt, *J* = 2.8, 8.4 Hz, 1H), 6.73 (dd, *J* = 2.8, 8.8 Hz, 1H), 5.28 (d, *J* = 1.6 Hz, 1H), 5.24 (t, *J* = 6.0 Hz, 1H), 5.19 (d, *J* = 2.0 Hz, 1H), 4.59 (td, *J* = 2.4, 14.4 Hz, 1H), 4.39 (td, *J* = 2.4, 14.4 Hz, 1H), 2.94 (s, 3H), 2.85 (dd, *J* = 6.0, 15.6 Hz, 1H), 2.79 (s, 3H), 2.65 (dd, *J* = 6.0, 15.2 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃) δ 169.3, 160.7, 159.6 (d, ¹J_{CF} = 241 Hz), 138.4, 135.7, 124.6 (d, ³J_{CF} = 8 Hz), 124.3 (d, ³J_{CF} = 8 Hz), 115.4 (d, ²J_{CF} = 22 Hz), 112.2 (d, ²J_{CF} = 24 Hz), 106.0, 56.7, 54.0, 39.0, 37.2, 35.6; HRMS calcd for C₁₅H₁₇FN₃OS⁺ (M + H⁺): 306.1071; Found: 306.1070.



N,N-dimethyl-2-(7-methyl-2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetamide(3sa)

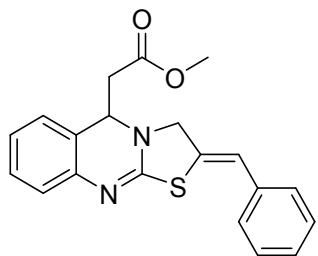
White oil; (52.5 mg, 87%); ¹H NMR (400 MHz, CDCl₃) δ 7.01 (d, *J* = 8.0 Hz, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.78 (s, 1H), 5.27 (d, *J* = 1.6 Hz, 1H), 5.17-5.21 (m, 2H), 4.60 (td, *J* = 2.0, 14.8 Hz, 1H), 4.38 (td, *J* = 2.0, 14.4 Hz, 1H), 2.92 (s, 3H), 2.84 (dd, *J* = 6.0, 15.2 Hz, 1H), 2.71 (s,

3H), 2.64 (dd, J = 6.0, 15.2 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 169.7, 160.5, 139.7, 136.0, 134.1, 129.4, 126.0, 123.1, 122.7, 105.8, 56.8, 54.4, 39.2, 37.3, 35.6, 20.9; HRMS calcd for $\text{C}_{16}\text{H}_{20}\text{N}_3\text{OS}^+$ ($\text{M} + \text{H}^+$): 302.1322; Found: 302.1324.



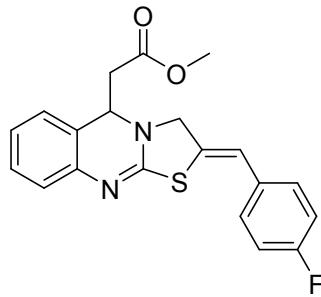
2-(2-methylene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetaldehyde (3ta)

Yellow solid; (26.9 mg, 55%); ^1H NMR (400 MHz, CDCl_3) δ 9.63 (s, 1H), 7.15 (t, J = 7.4 Hz, 1H), 7.08 (d, J = 7.2 Hz, 1H), 7.00 (t, J = 7.6 Hz, 1H), 6.86 (d, J = 8.0 Hz, 1H), 5.38 (d, J = 1.6 Hz, 1H), 5.30 (d, J = 1.2 Hz, 1H), 5.25 (t, J = 4.6 Hz, 1H), 4.62 (d, J = 14.8 Hz, 1H), 4.38 (d, J = 14.8 Hz, 1H), 3.05-3.10 (m, 1H), 2.90-2.96 (m, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 201.4, 142.4, 135.7, 128.9, 126.4, 124.7, 123.4, 123.1, 122.8, 106.8, 56.6, 52.4, 48.9; HRMS calcd for $\text{C}_{13}\text{H}_{13}\text{N}_2\text{OS}^+$ ($\text{M} + \text{H}^+$): 245.0743; Found: 245.0745.



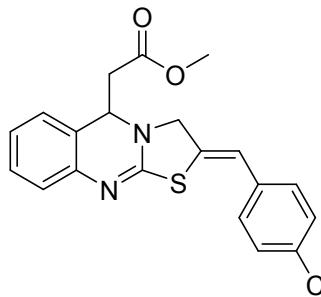
methyl (Z)-2-(2-benzylidene-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate (3ab)

Yellow solid; (63.1 mg, 90%); ^1H NMR (400 MHz, CDCl_3) δ 7.38 (t, J = 7.6 Hz, 2H), 7.30 (d, J = 7.2 Hz, 2H), 7.27-7.20 (m, 2H), 7.09 (dd, J = 0.8, 8.0 Hz, 1H), 7.04 (dt, J = 1.2, 7.6 Hz, 1H), 6.98 (dd, J = 1.2, 7.6 Hz, 1H), 6.58 (s, 1H), 5.21 (t, J = 5.6 Hz, 1H), 4.76 (dd, J = 2.0, 14.4 Hz, 1H), 4.51 (dd, J = 2.0, 14.4 Hz, 1H), 3.67 (s, 3H), 2.89-2.74 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.0, 160.9, 141.8, 135.5, 129.1, 128.7, 127.8, 127.4, 126.5, 125.5, 124.8, 123.8, 121.8, 120.6, 58.1, 54.3, 52.2, 40.5; HRMS calcd for $\text{C}_{20}\text{H}_{19}\text{N}_2\text{O}_2\text{S}^+$ ($\text{M} + \text{H}^+$): 351.1162; Found: 351.1168.



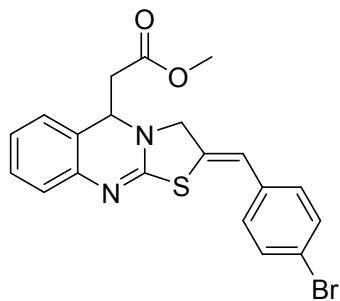
methyl (Z)-2-(2-(4-fluorobenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ac)

Yellow solid; (59.7 mg, 81%); ¹H NMR (400 MHz, CDCl₃) δ 7.19-7.11 (m, 3H), 7.00-6.93 (m, 4H), 6.88 (d, *J* = 7.2 Hz, 1H), 6.44 (s, 1H), 5.09 (t, *J* = 5.6 Hz, 1H), 4.64 (d, *J* = 14.4 Hz, 1H), 4.38 (d, *J* = 14.4 Hz, 1H), 3.57 (s, 3H), 2.78-2.64 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 171.0, 161.7 (d, ¹J_{CF} = 247 Hz), 160.4, 141.9, 131.8 (d, ⁴J_{CF} = 3 Hz), 129.4 (d, ³J_{CF} = 8 Hz), 129.1, 126.4, 125.6, 124.8, 123.9, 121.8, 119.4, 115.7 (d, ²J_{CF} = 21 Hz), 58.0, 54.2, 52.2, 40.5; HRMS calcd for C₂₀H₁₈FN₂O₂S⁺ (M + H⁺): 369.1068; Found: 369.1067.



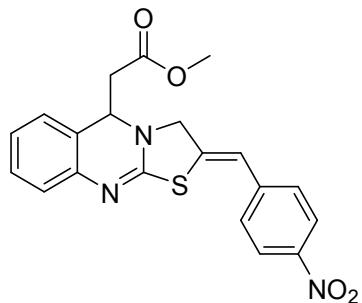
methyl (Z)-2-(2-(4-chlorobenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ad)

Yellow solid; (63.9 mg, 83%); ¹H NMR (400 MHz, CDCl₃) δ 7.24 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 3H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.95 (t, *J* = 7.6 Hz, 1H), 6.88 (t, *J* = 7.6 Hz, 1H), 6.42 (s, 1H), 5.09 (t, *J* = 5.2 Hz, 1H), 4.64 (dd, *J* = 1.6, 14.4 Hz, 1H), 4.38 (dd, *J* = 1.6, 14.4 Hz, 1H), 3.57 (s, 3H), 2.78-2.64 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 170.9, 160.5, 141.7, 134.0, 132.9, 129.1, 129.0, 128.9, 127.5, 125.6, 124.9, 123.8, 121.8, 119.4, 58.0, 54.2, 52.2, 40.4; HRMS calcd for C₂₀H₁₈ClN₂O₂S⁺ (M + H⁺): 385.0772; Found: 385.0787.



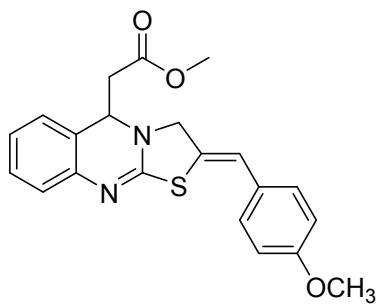
methyl (Z)-2-(2-(4-bromobenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ae)

Yellow solid; (61.0 mg, 81%); ^1H NMR (400 MHz, CDCl_3) δ 7.39 (d, $J = 8.8$ Hz, 2H), 7.13 (t, $J = 7.2$ Hz, 1H), 7.06 (d, $J = 8.4$ Hz, 2H), 7.00 (d, $J = 7.6$ Hz, 1H), 6.95 (t, $J = 7.6$ Hz, 1H), 6.88 (d, $J = 7.2$ Hz, 1H), 6.39 (s, 1H), 5.08 (t, $J = 5.2$ Hz, 1H), 4.63 (dd, $J = 1.6, 14.4$ Hz, 1H), 4.36 (dd, $J = 1.6, 14.8$ Hz, 1H), 3.57 (s, 3H), 2.78-2.64 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.9, 160.5, 141.7, 134.5, 131.8, 129.3, 129.1, 127.6, 125.6, 124.9, 123.8, 121.8, 121.1, 119.4, 58.1, 54.2, 52.2, 40.4; HRMS calcd for $\text{C}_{20}\text{H}_{18}\text{BrN}_2\text{O}_2\text{S}^+(\text{M} + \text{H}^+)$: 429.0267; Found: 429.0293.



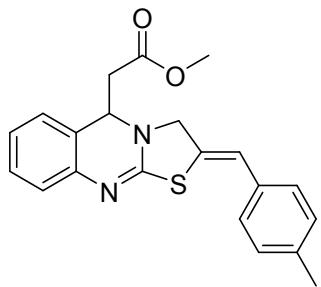
methyl (Z)-2-(2-(4-nitrobenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3af)

Yellow solid; (50.6 mg, 64%); ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, $J = 8.4$ Hz, 2H), 7.42 (d, $J = 8.8$ Hz, 2H), 7.23 (t, $J = 7.6$ Hz, 1H), 7.05-7.10 (m, 2H), 6.99 (d, $J = 7.6$ Hz, 1H), 6.62 (s, 1H), 5.22 (t, $J = 5.2$ Hz, 1H), 4.83 (d, $J = 15.2$ Hz, 1H), 4.57 (d, $J = 15.2$ Hz, 1H), 3.67 (s, 3H), 2.89-2.76 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.9, 159.7, 146.1, 142.0, 141.6, 132.8, 129.2, 128.3, 125.6, 125.2, 124.1, 124.0, 121.7, 118.3, 58.4, 54.3, 52.2, 40.5; HRMS calcd for $\text{C}_{20}\text{H}_{18}\text{N}_3\text{O}_4\text{S}^+(\text{M} + \text{H}^+)$: 396.1013; Found: 396.1012.



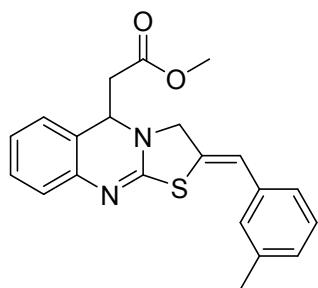
methyl (Z)-2-(2-(4-methoxybenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ag)

Yellow solid; (68.5 mg, 90%); ^1H NMR (400 MHz, CDCl_3) δ 7.14 (q, $J = 8.8$ Hz, 3H), 6.99 (d, $J = 7.6$ Hz, 1H), 6.94 (t, $J = 7.6$ Hz, 1H), 6.87 (d, $J = 7.2$ Hz, 1H), 6.81 (d, $J = 8.4$ Hz, 1H), 6.41 (s, 1H), 5.07 (t, $J = 5.2$ Hz, 1H), 4.61 (d, $J = 14.8$ Hz, 1H), 4.34 (d, $J = 14.0$ Hz, 1H), 3.71 (s, 3H), 3.56 (s, 3H), 2.77-2.63 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.9, 160.1, 158.7, 142.0, 129.1, 129.0, 128.2, 125.5, 124.7, 123.8, 121.8, 120.2, 114.2, 58.0, 55.3, 54.2, 52.1, 40.4; HRMS calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}_3\text{S}^+(\text{M} + \text{H}^+)$: 381.1267; Found: 381.1288.



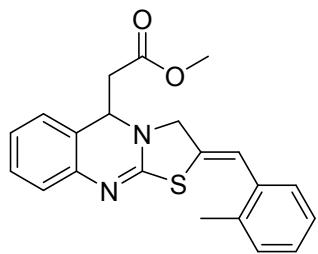
methyl (Z)-2-(2-(4-methylbenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ah)

Yellow solid; (68.2 mg, 94%); ^1H NMR (400 MHz, CDCl_3) δ 7.16-7.09 (m, 5H), 7.01 (d, $J = 6.8$ Hz, 1H), 6.95 (dt, $J = 0.8, 7.6$ Hz, 1H), 6.89 (d, $J = 7.2$ Hz, 1H), 6.46 (s, 1H), 5.11 (t, $J = 5.6$ Hz, 1H), 4.65 (d, $J = 14.8$ Hz, 1H), 4.40 (d, $J = 14.4$ Hz, 1H), 3.58 (s, 3H), 2.80-2.65 (m, 2H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.0, 161.1, 141.8, 137.3, 132.7, 129.5, 129.1, 127.8, 125.5, 125.2, 124.7, 123.8, 121.8, 120.6, 58.1, 54.2, 52.1, 40.5, 21.3; HRMS calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+(\text{M} + \text{H}^+)$: 365.1318; Found: 365.1319



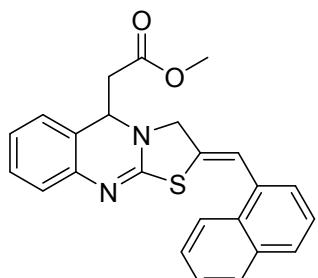
methyl (Z)-2-(2-(3-methylbenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3ai)

Yellow solid; (67.1 mg, 92%); ^1H NMR (400 MHz, CDCl_3) δ 7.19 (q, $J = 7.6$ Hz, 1H), 7.13 (d, $J = 7.6$ Hz, 1H), 7.04-6.94 (m, 5H), 6.89 (d, $J = 7.2$ Hz, 1H), 6.46 (s, 1H), 5.12 (t, $J = 5.4$ Hz, 1H), 4.66 (d, $J = 14.4$ Hz, 1H), 4.41 (d, $J = 14.0$ Hz, 1H), 3.59 (s, 3H), 2.80-2.65 (m, 2H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.0, 161.0, 141.9, 138.4, 135.5, 129.1, 128.6, 128.5, 128.2, 126.3, 125.5, 124.9, 124.7, 123.9, 121.9, 120.7, 58.1, 54.2, 52.2, 40.5, 21.5; HRMS calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+(\text{M} + \text{H}^+)$: 365.1318; Found: 365.1339.



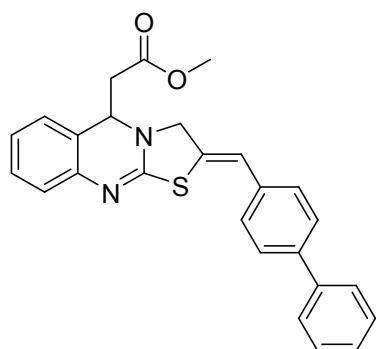
methyl (Z)-2-(2-(2-methylbenzylidene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate(3aj)

Yellow solid; (65.6 mg, 90%); ^1H NMR (400 MHz, CDCl_3) δ 7.26 (d, $J = 7.2$ Hz, 1H), 7.19-7.11 (m, 4H), 7.02 (d, $J = 7.6$ Hz, 1H), 6.96 (t, $J = 7.2$ Hz, 1H), 6.91 (d, $J = 7.2$ Hz, 1H), 6.62 (s, 1H), 5.15 (t, $J = 4.8$ Hz, 1H), 4.70 (d, $J = 14.4$ Hz, 1H), 4.47 (d, $J = 14.4$ Hz, 1H), 3.60 (s, 3H), 2.84-2.68 (m, 2H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 171.1, 161.1, 149.4, 141.4, 136.0, 134.7, 130.3, 129.1, 127.8, 126.9, 126.2, 125.5, 124.8, 123.6, 121.7, 119.2, 57.7, 54.3, 52.2, 40.5, 19.9; HRMS calcd for $\text{C}_{21}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+(\text{M} + \text{H}^+)$: 365.1318; Found: 365.1349.



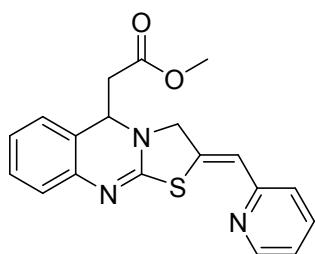
methyl (Z)-2-(2-(naphthalen-1-ylmethylene)-2,3-dihydro-5H-thiazolo[2,3-*b*]quinazolin-5-yl)acetate(3ak)

Yellow solid; (75.3 mg, 94%); ¹H NMR (400 MHz, CDCl₃) δ 7.95-7.93 (m, 1H), 7.84-7.82 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.51-7.44 (m, 4H), 7.19 (t, *J* = 8.4 Hz, 1H), 7.13 (s, 1H), 7.08 (d, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 6.8 Hz, 1H), 5.15 (t, *J* = 5.6 Hz, 1H), 4.79 (dd, *J* = 2.0, 14.4 Hz, 1H), 4.50 (dd, *J* = 2.0, 14.4 Hz, 1H), 3.65 (s, 3H), 2.87-2.72 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 171.0, 160.9, 141.9, 133.7, 133.0, 131.1, 130.0, 129.1, 128.7, 128.4, 126.3, 126.2, 125.6, 125.5, 125.3, 124.7, 123.8, 123.7, 121.9, 117.9, 57.5, 54.3, 52.2, 40.5; HRMS calcd for C₂₄H₂₁N₂O₂S⁺(M + H⁺): 401.1318; Found: 401.1318.



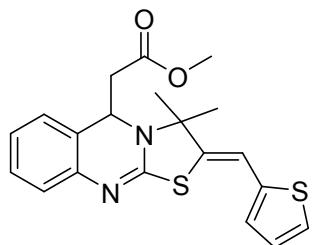
methyl (Z)-2-(2-(1,1'-biphenyl)-4-ylmethylene)-2,3-dihydro-5H-thiazolo[2,3-*b*]quinazolin-5-yl)acetate (3al)

Yellow solid; (69.1 mg, 81%); ¹H NMR (400 MHz, CDCl₃) δ 7.61-7.58 (m, 4H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.36-7.31 (m, 3H), 7.22 (t, *J* = 10.4 Hz, 1H), 7.10 (d, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.94 (d, *J* = 7.2 Hz, 1H), 6.56 (s, 1H), 5.15 (t, *J* = 5.6 Hz, 1H), 4.72 (dd, *J* = 1.6, 14.4 Hz, 1H), 4.45 (dd, *J* = 1.6, 14.4 Hz, 1H), 3.64 (s, 3H), 2.84-2.71 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 171.0, 160.9, 141.9, 140.3, 139.9, 134.6, 129.1, 128.9, 128.3, 127.5, 127.3, 127.0, 126.6, 125.6, 124.8, 123.9, 121.9, 120.2, 58.1, 54.3, 52.2, 40.5; HRMS calcd for C₂₆H₂₃N₂O₂S⁺(M + H⁺): 427.1475; Found: 427.1477.



methyl (Z)-2-(2-(pyridin-2-ylmethylene)-2,3-dihydro-5H-thiazolo[2,3-*b*]quinazolin-5-yl)acetate(3am)

Yellow solid; (49.2 mg, 70%); ^1H NMR (400 MHz, CDCl_3) δ 8.55 (s, 1H), 8.46 (d, $J = 4.4$ Hz, 1H), 7.64 (d, $J = 7.6$ Hz, 1H), 7.34-7.29 (m, 1H), 7.23 (t, $J = 7.6$ Hz, 1H), 7.07 (q, $J = 8.0$ Hz, 2H), 6.98 (d, $J = 7.6$ Hz, 1H), 6.54 (s, 1H), 5.21 (t, $J = 5.2$ Hz, 1H), 4.80 (d, $J = 14.4$ Hz, 1H), 4.54 (d, $J = 1.6, 14.8$ Hz, 1H), 3.67 (s, 3H), 2.89-2.75 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.9, 160.1, 149.6, 148.0, 141.7, 133.9, 131.5, 129.8, 129.1, 125.5, 125.0, 123.9, 123.5, 121.8, 116.8, 58.2, 54.3, 52.2, 40.5; HRMS calcd for $\text{C}_{19}\text{H}_{18}\text{N}_3\text{O}_2\text{S}^+$ ($M + \text{H}^+$): 352.1114; Found: 352.1114.



methyl (Z)-2-(3,3-dimethyl-2-(thiophen-2-ylmethylene)-2,3-dihydro-5H-thiazolo[2,3-b]quinazolin-5-yl)acetate (3an)

Yellow solid; (66.1 mg, 86%); ^1H NMR (400 MHz, CDCl_3) δ 7.27-7.26 (m, 1H), 7.18-7.13 (m, 1H), 7.07 (d, $J = 7.6$ Hz, 1H), 6.99-6.97 (m, 2H), 6.94 (d, $J = 3.6$ Hz, 2H), 6.67 (s, 1H), 5.07 (dd, $J = 2.4, 9.2$ Hz, 1H), 3.52 (s, 3H), 2.72-2.67 (m, 1H), 2.50 (dd, $J = 5.2, 15.2$ Hz, 1H), 1.68 (s, 3H), 1.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 170.5, 158.2, 142.8, 139.8, 136.5, 129.0, 127.5, 126.9, 126.1, 125.1, 124.4, 123.6, 123.1, 112.6, 70.3, 51.9, 51.2, 44.1, 29.4, 27.7; HRMS calcd for $\text{C}_{20}\text{H}_{21}\text{N}_2\text{O}_2\text{S}^+$ ($M + \text{H}^+$): 385.1039; Found: 385.1029.

3. X-Ray Crystal Structure for Compound 3ab

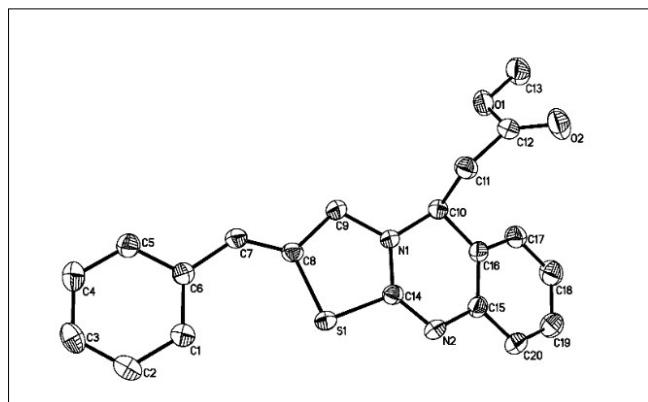
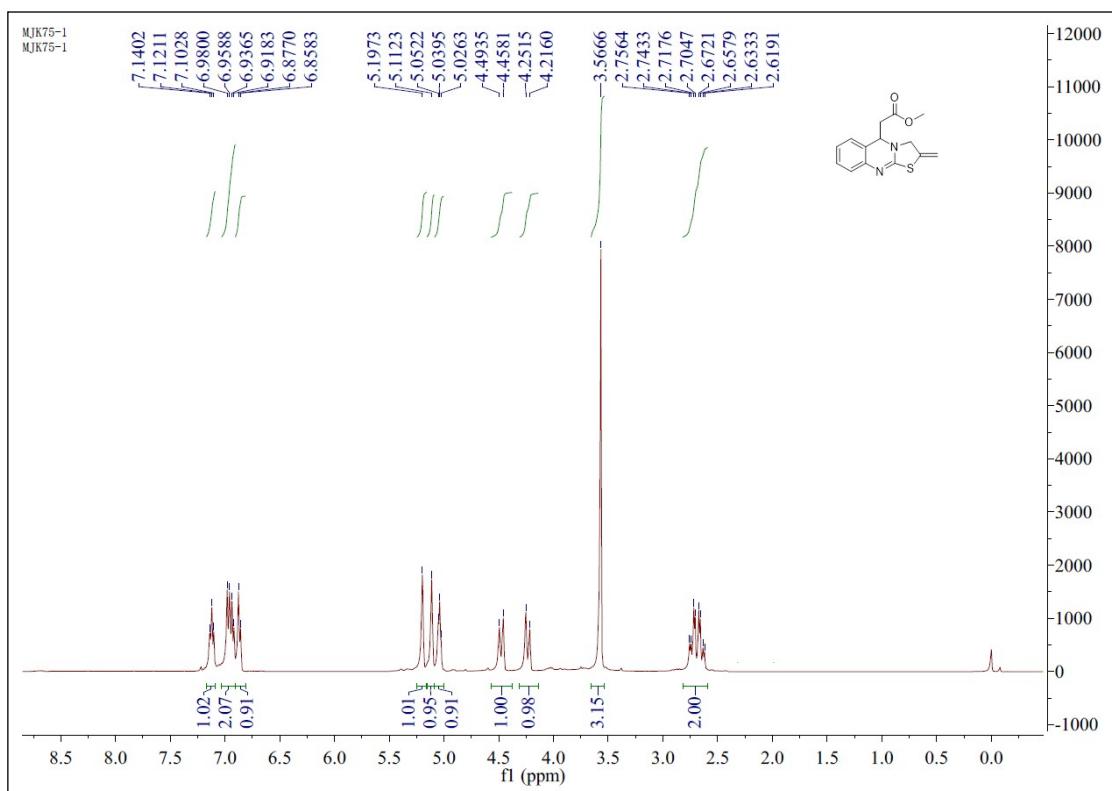


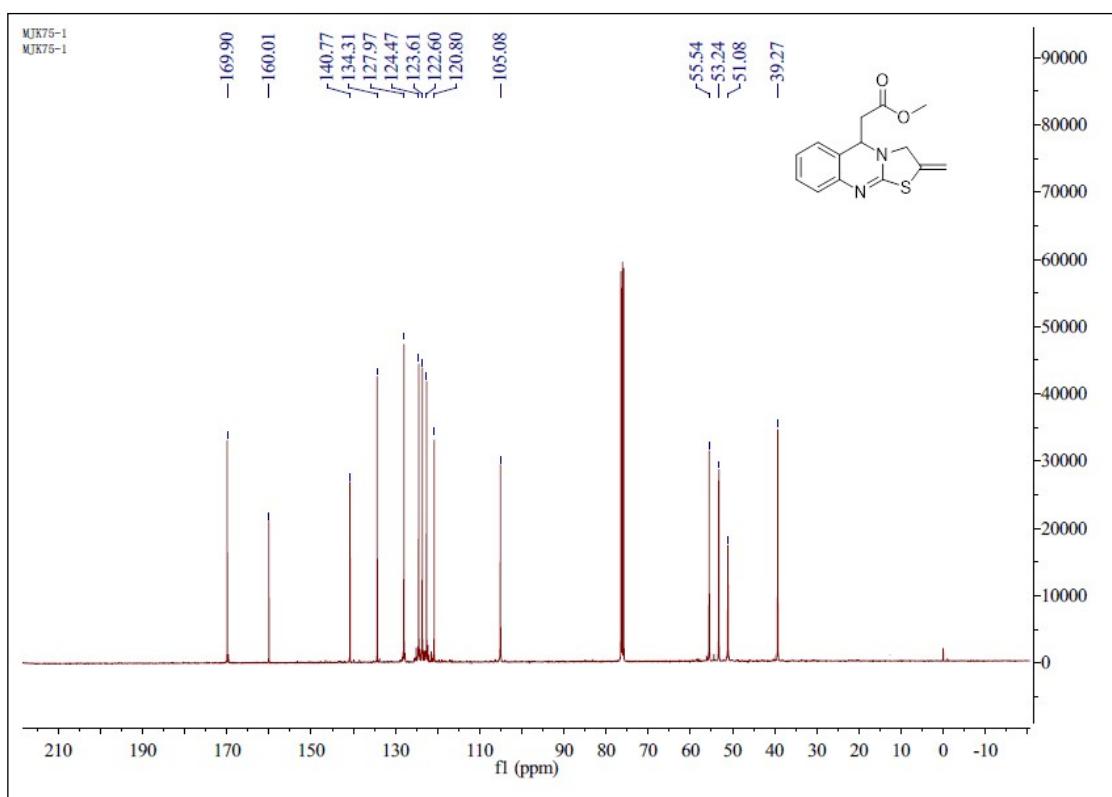
Figure 1. Single-crystal X-ray diffraction structure of **3ab**, the thermal ellipsoids are at the 30% probability level

CCDC: 1908021

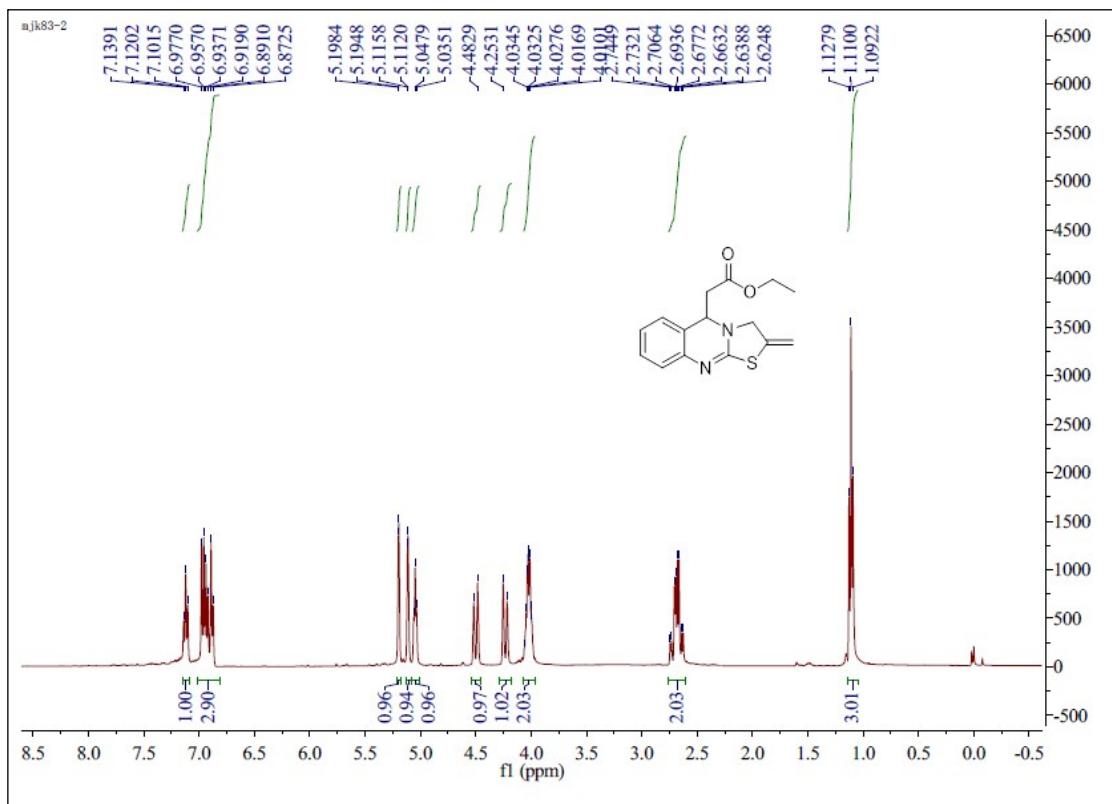
¹H NMR of **3aa**



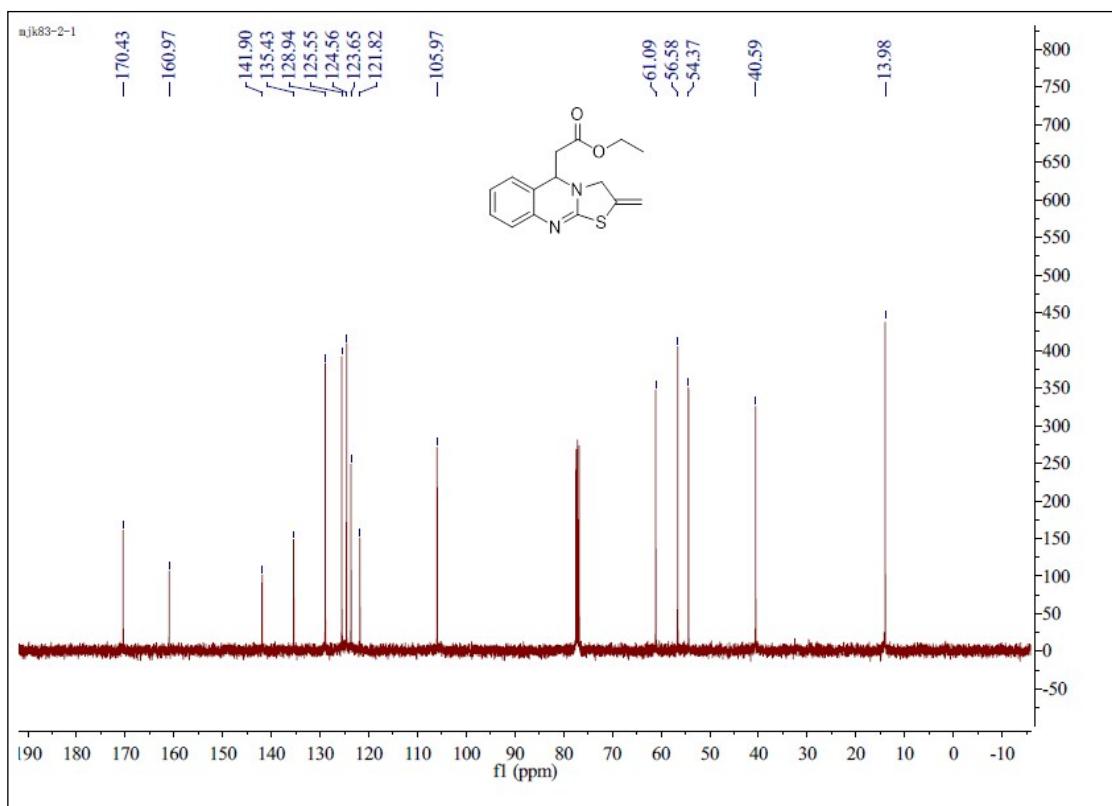
¹³C NMR of **3aa**



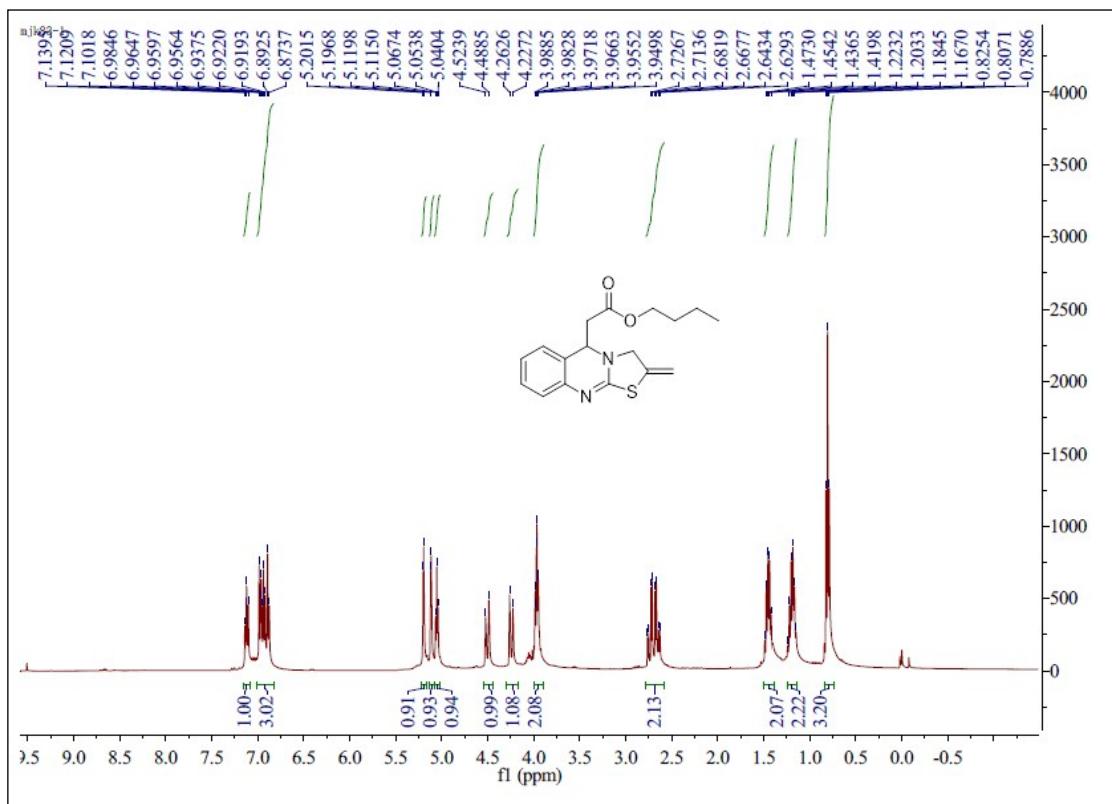
¹H NMR of 3ba



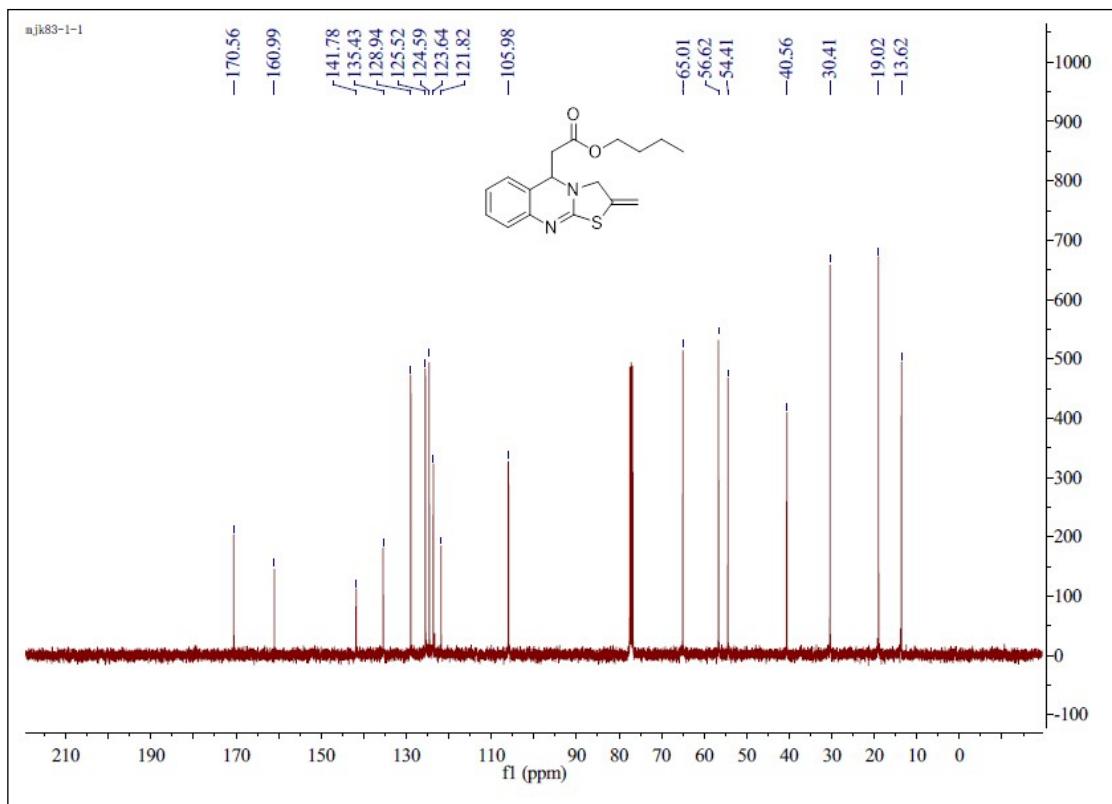
¹³C NMR of 3ba



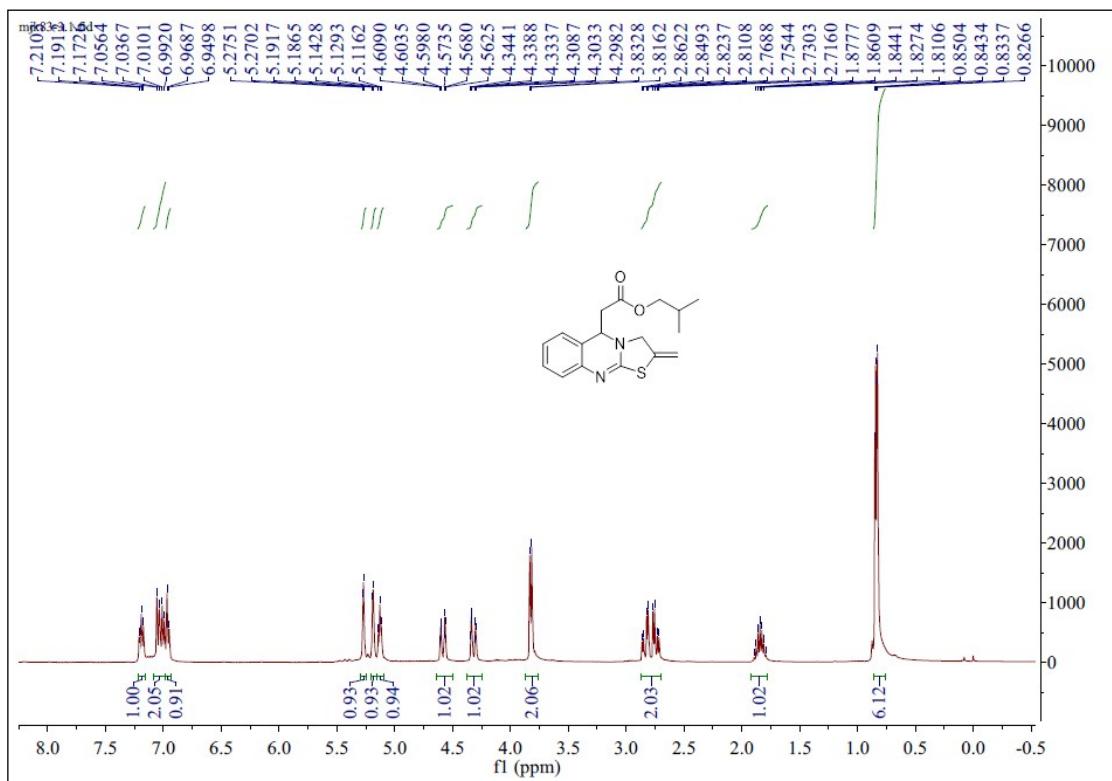
¹H NMR of 3ca



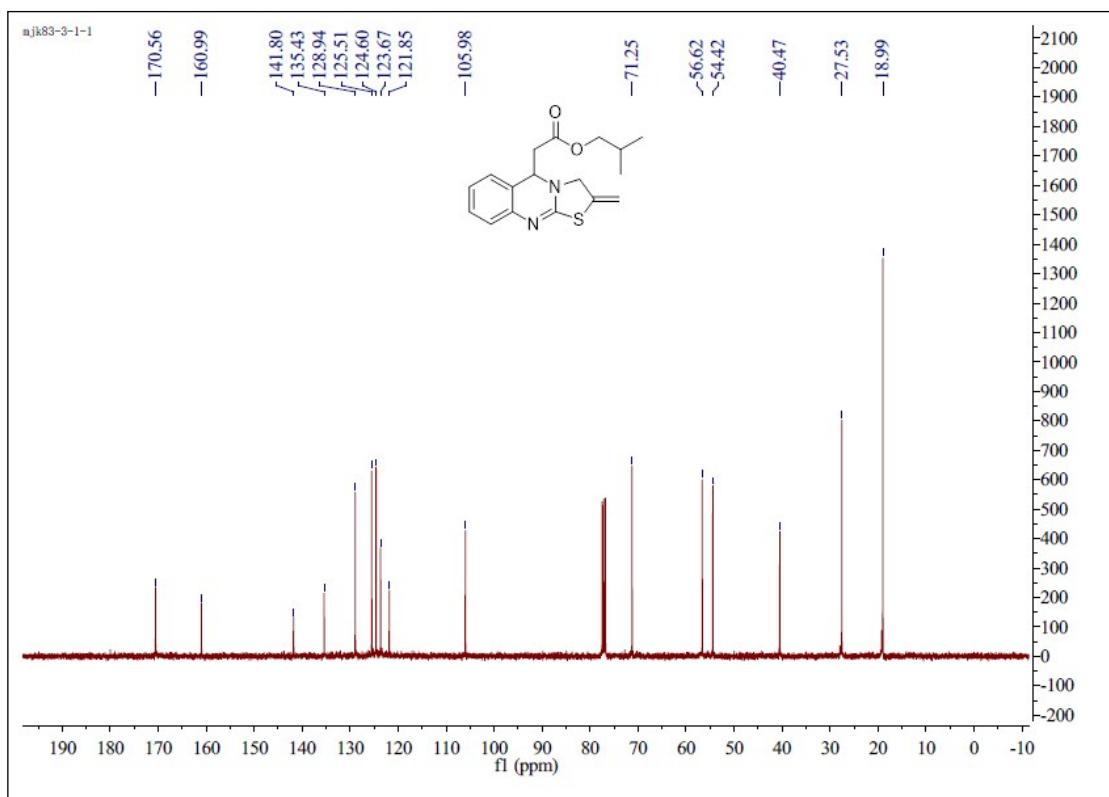
¹³C NMR of 3ca



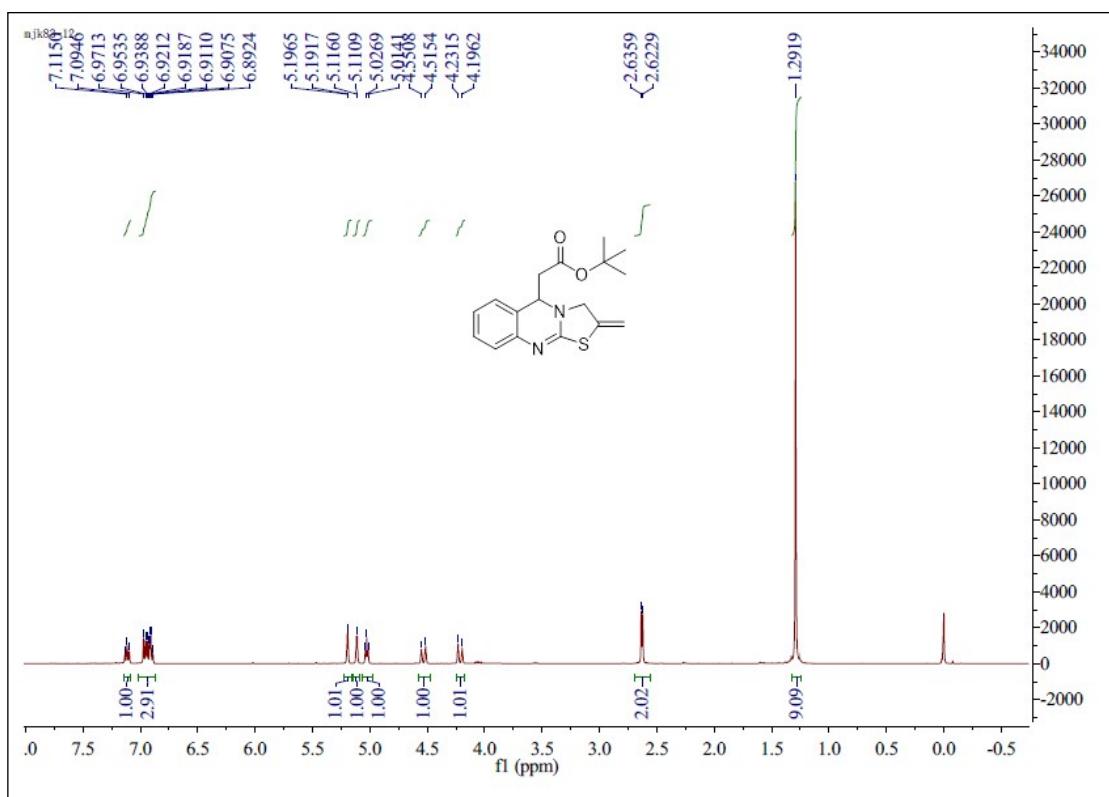
¹H NMR of 3da



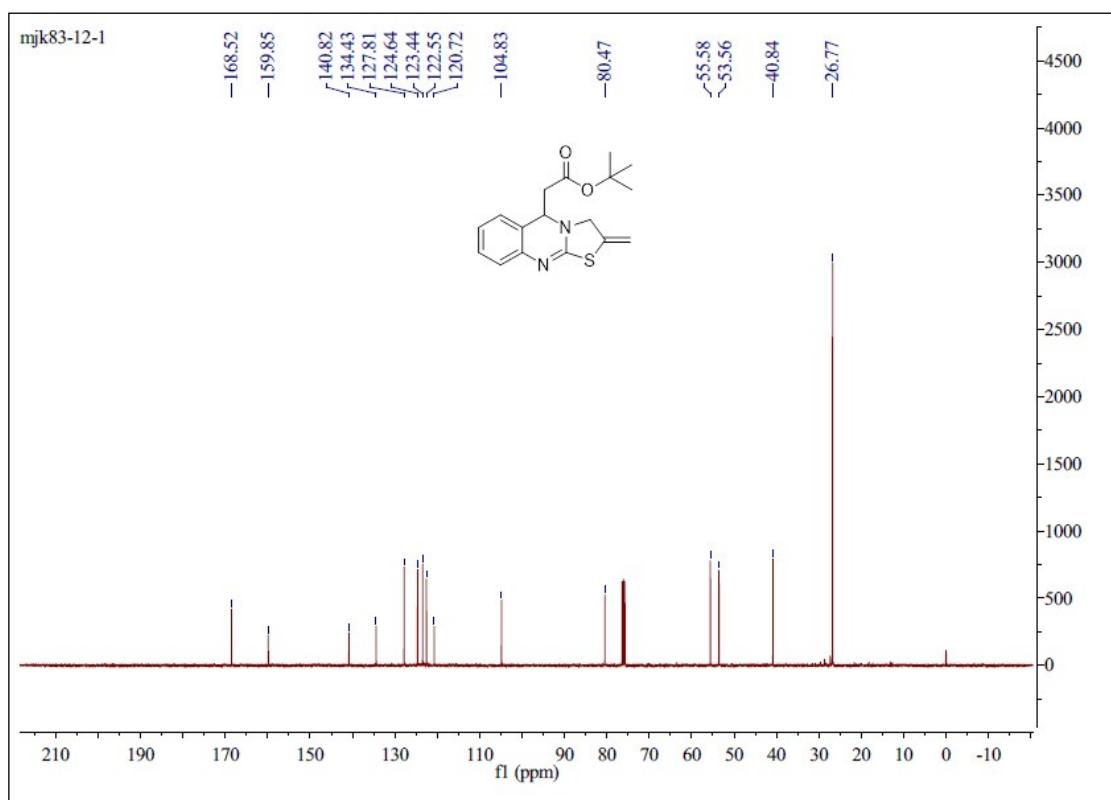
¹³C NMR of 3da



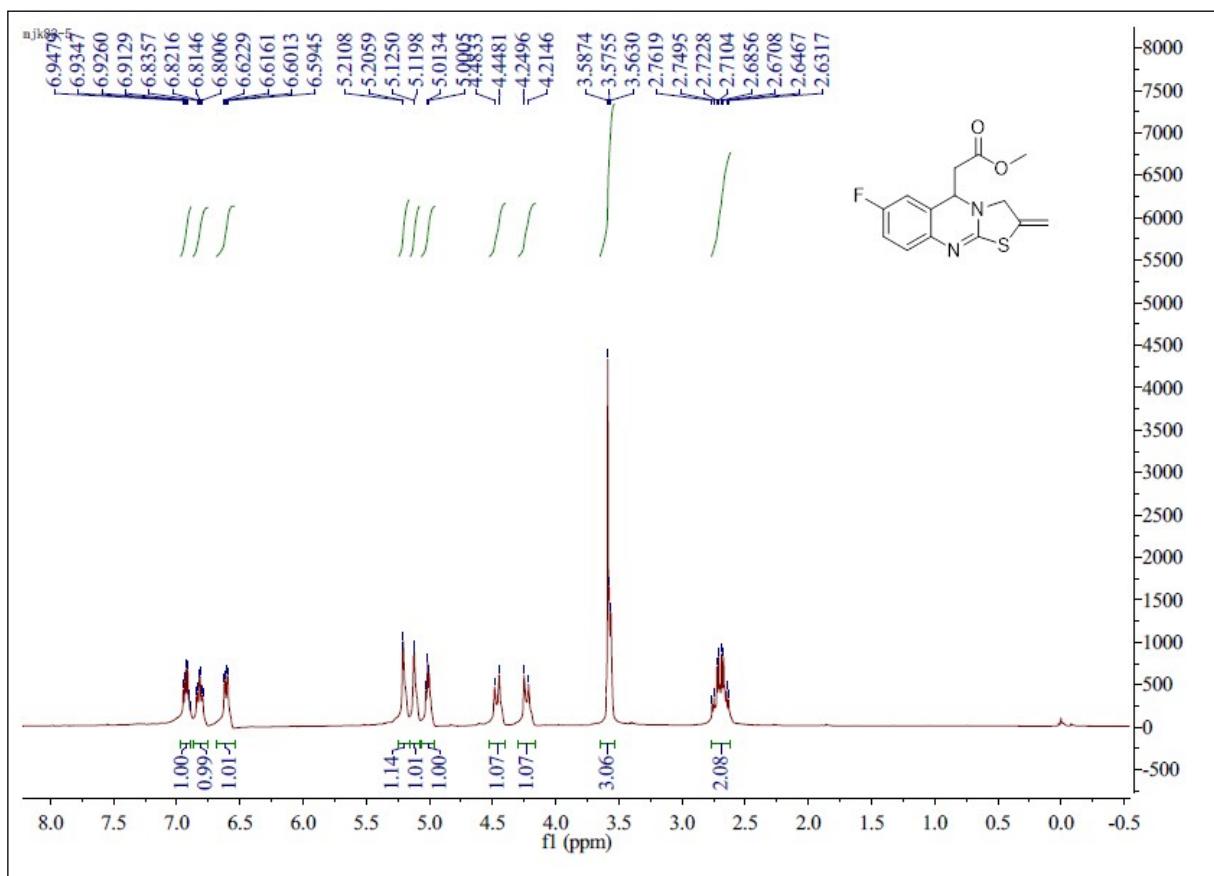
¹H NMR of 3ea



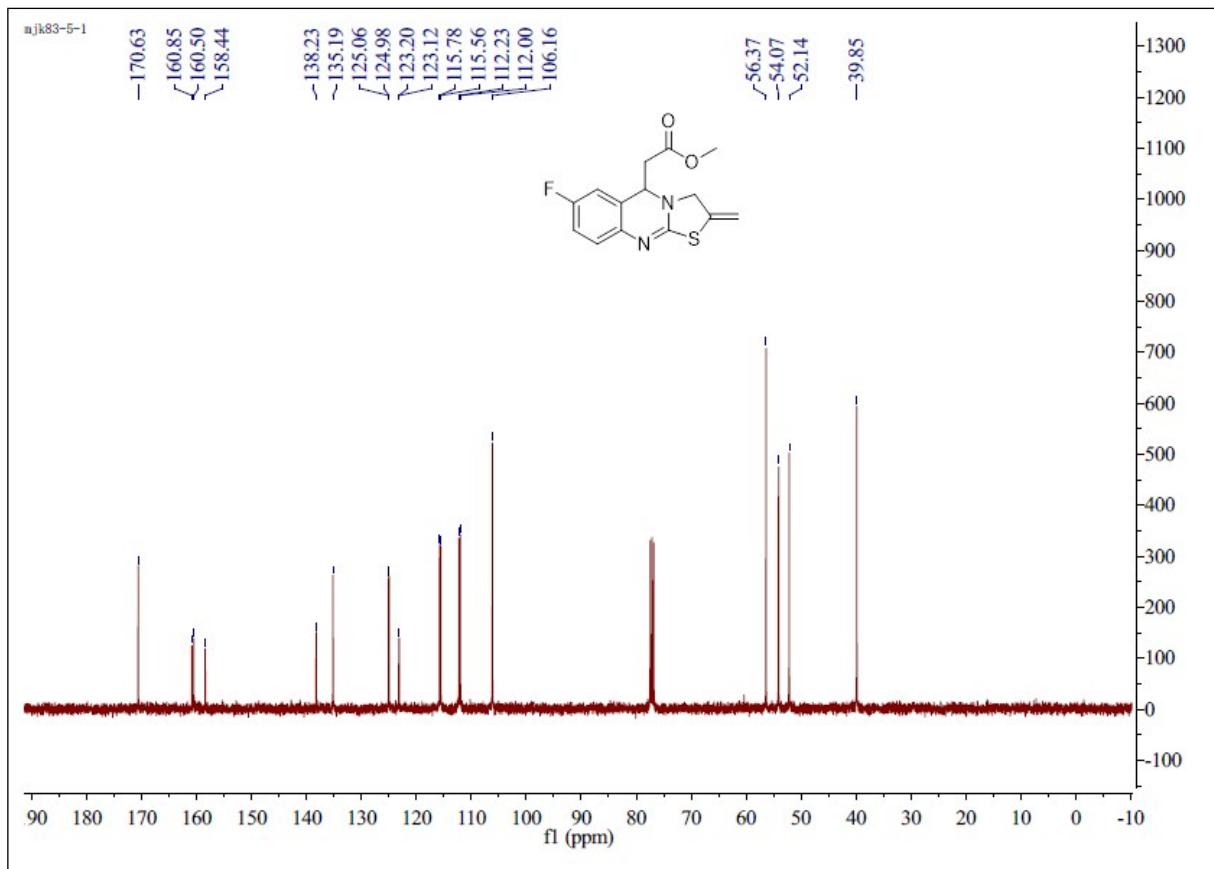
¹³C NMR of 3ea



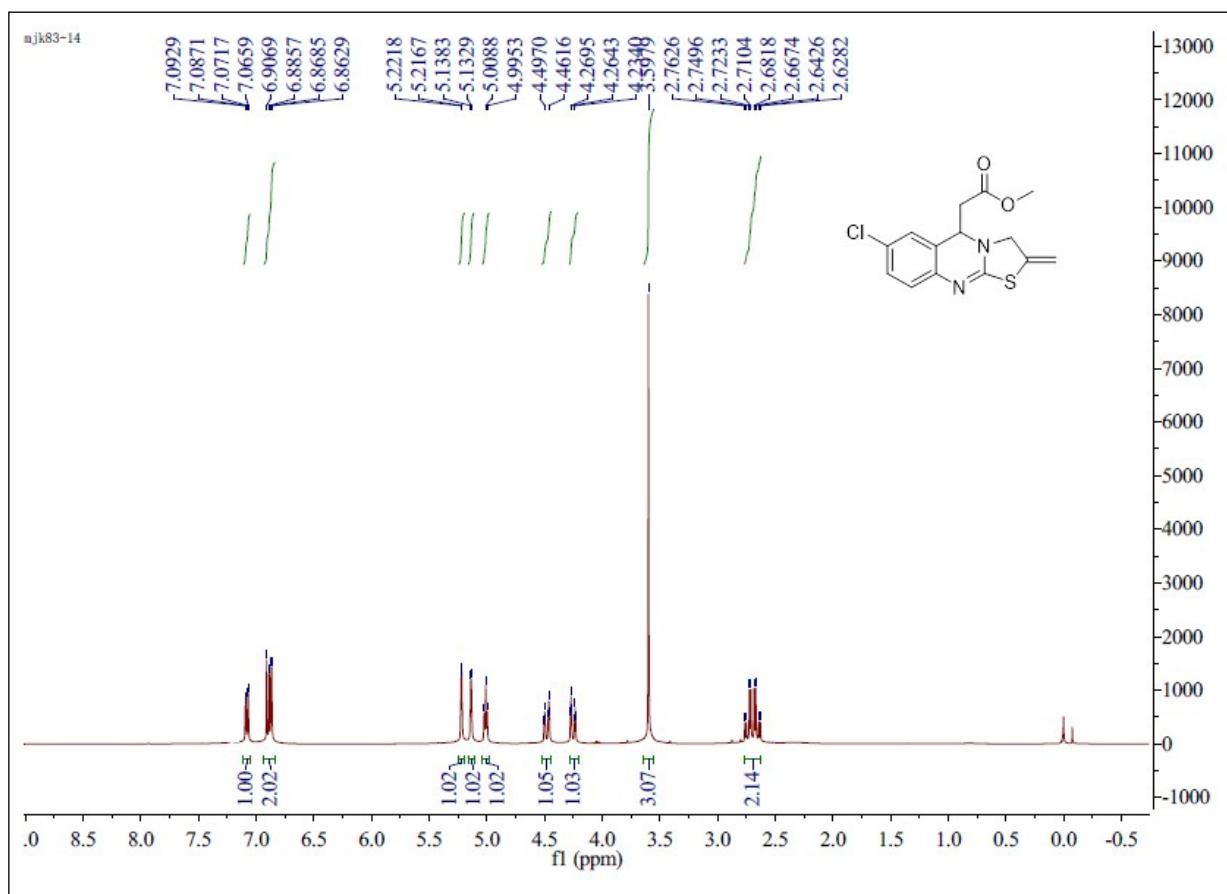
¹H NMR of 3fa



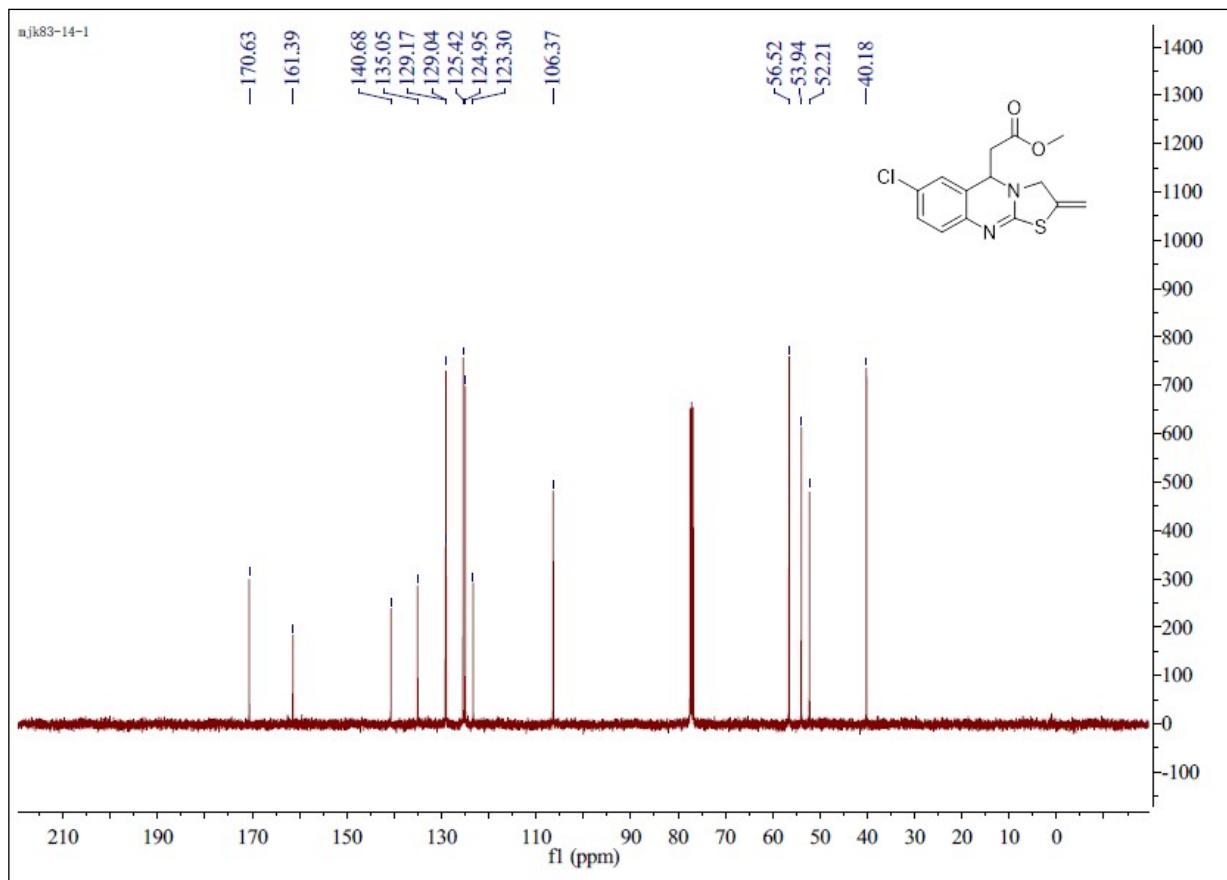
¹³C NMR of 3fa



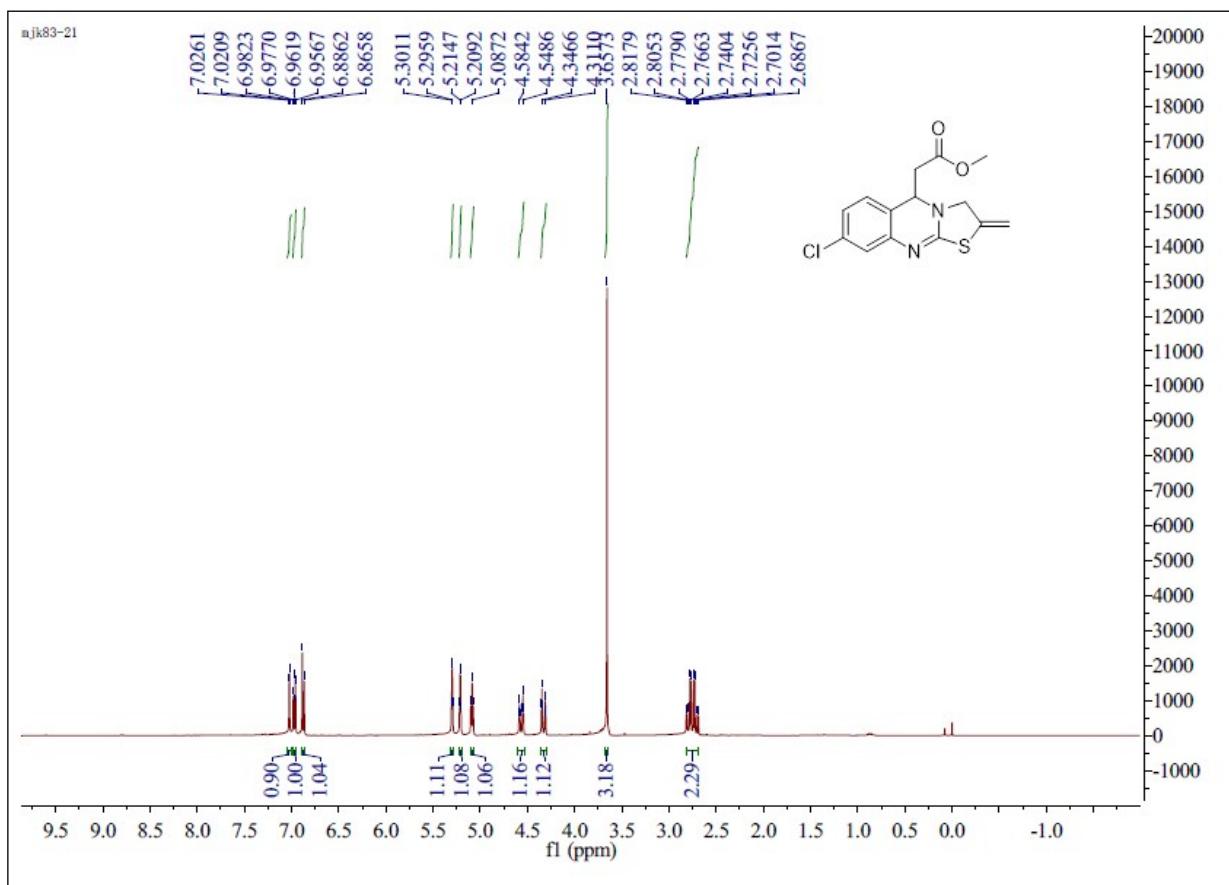
¹H NMR of 3ga



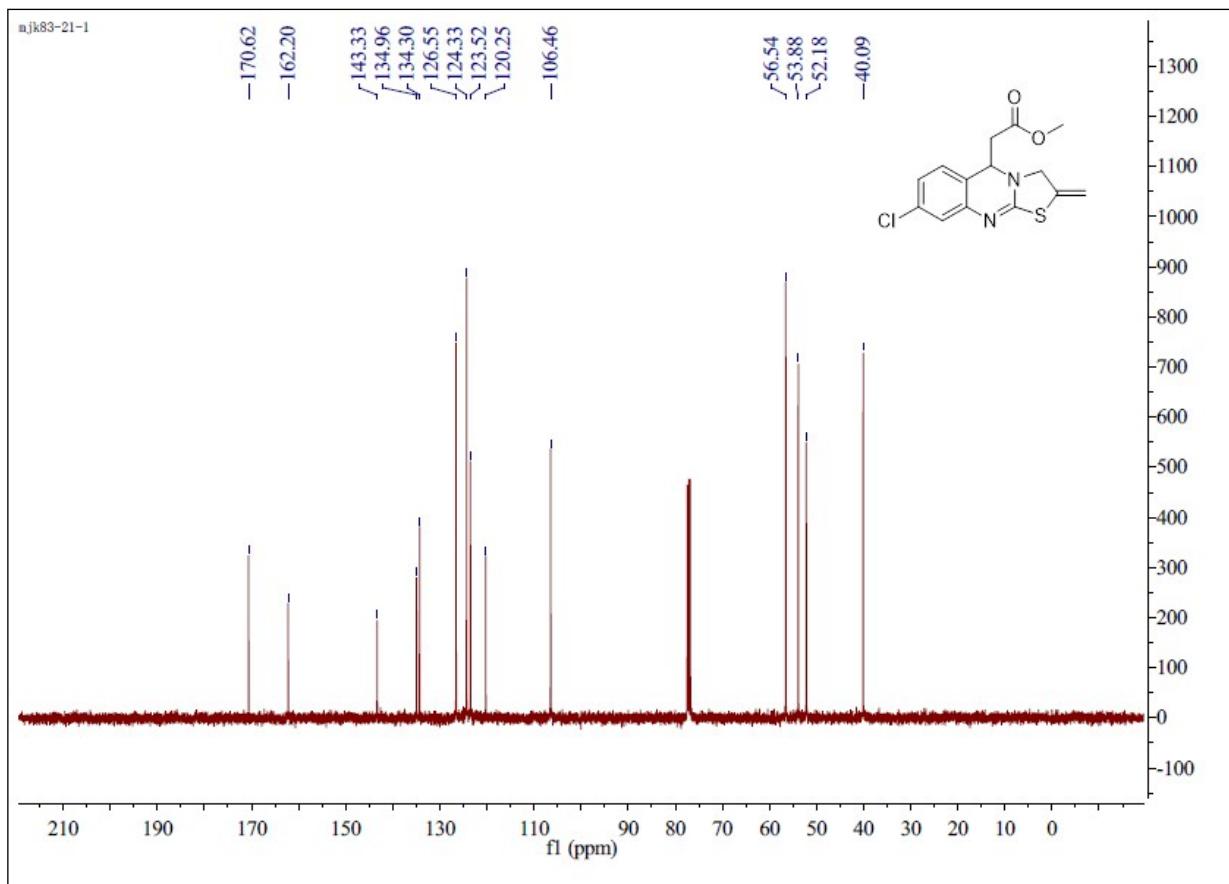
¹³C NMR of 3ga



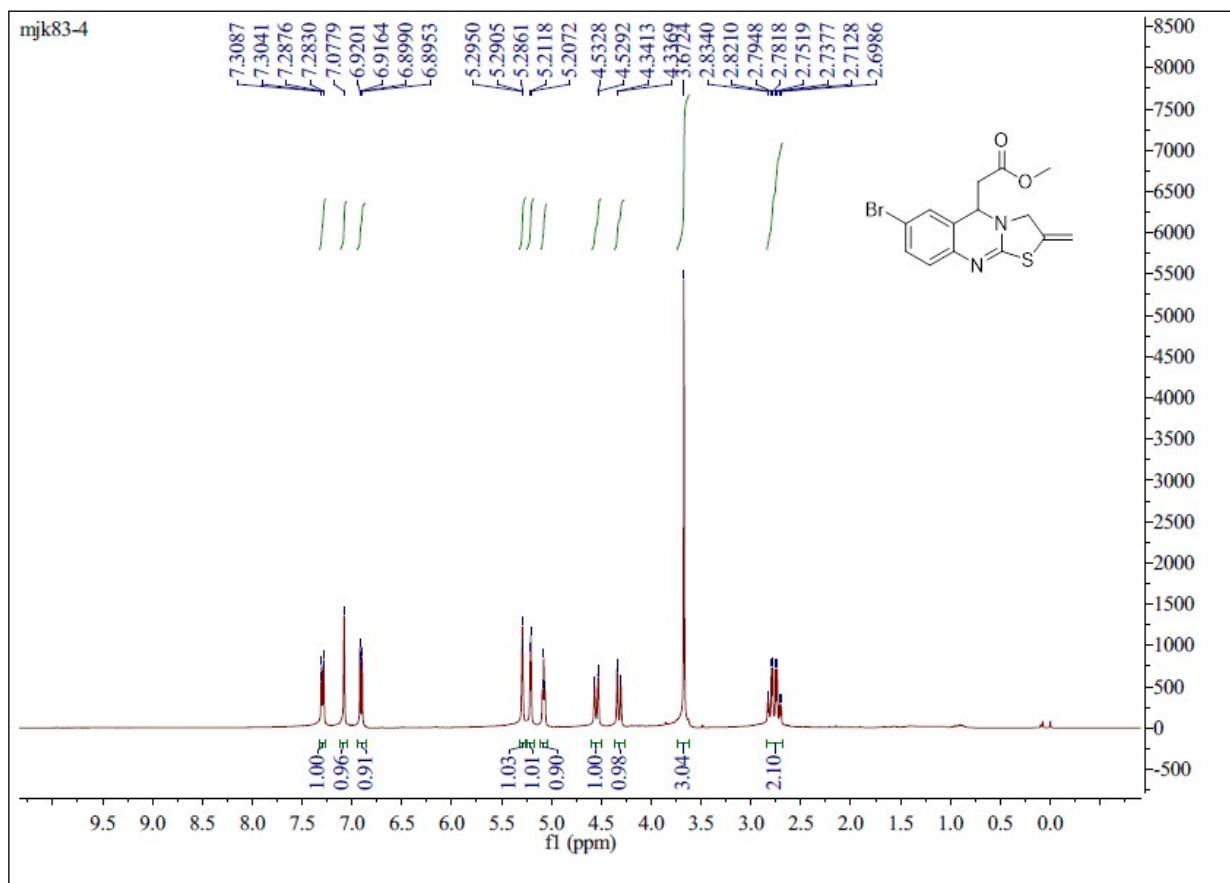
¹H NMR of 3ha



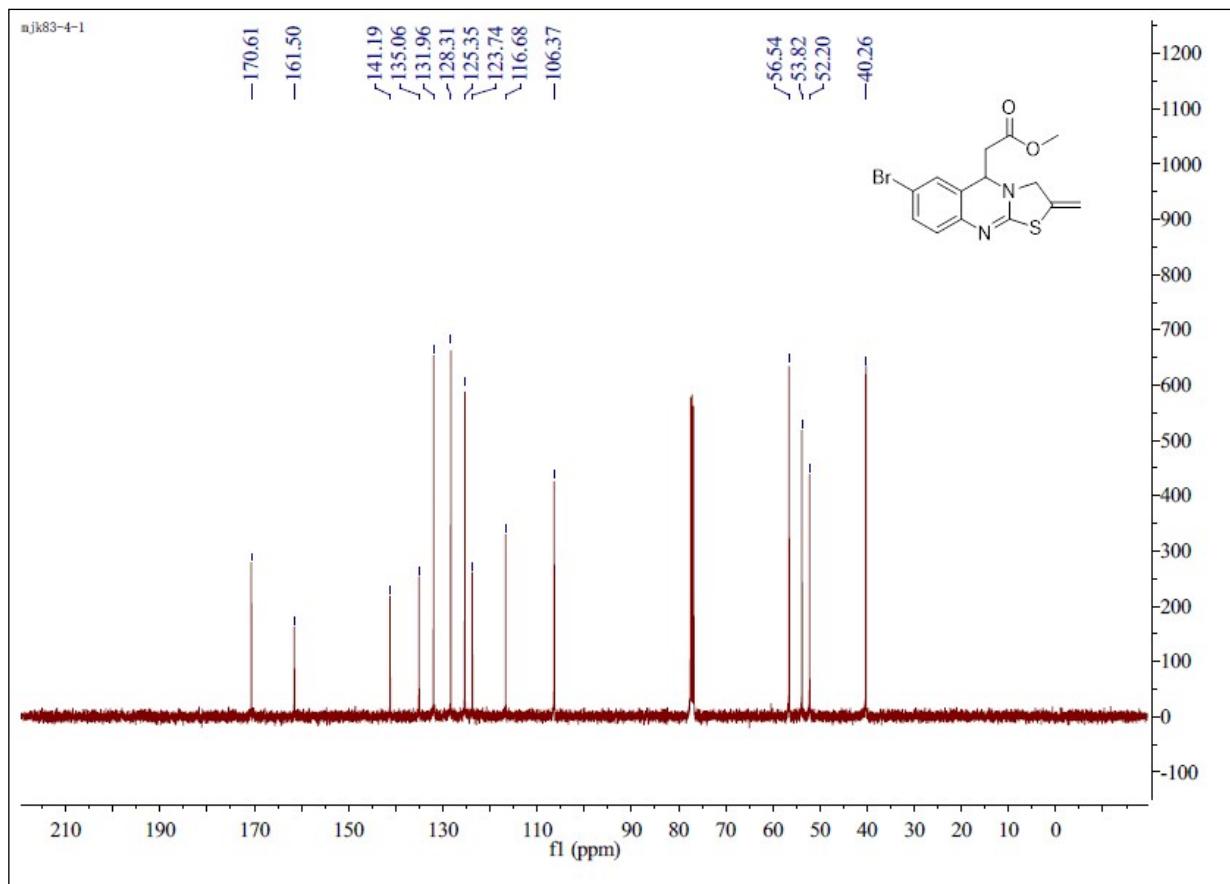
¹³C NMR of **3ha**



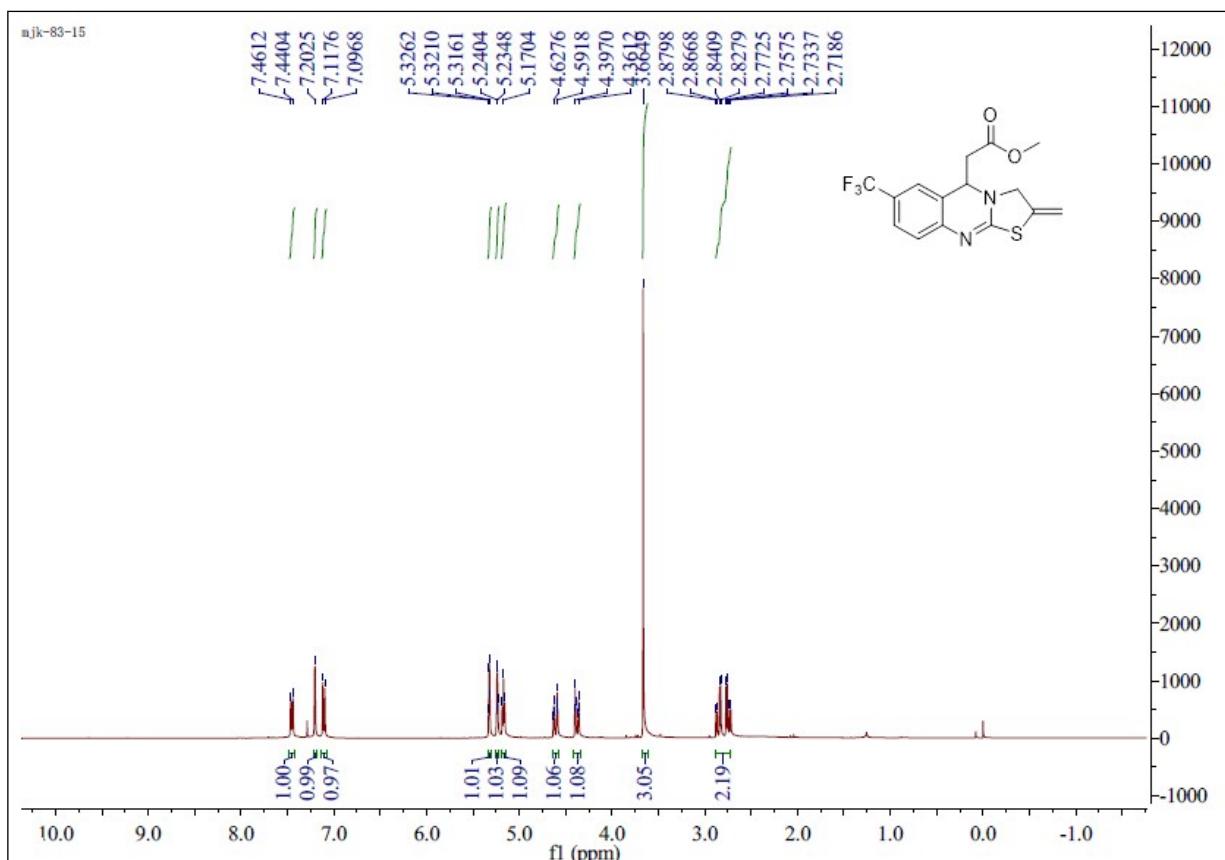
¹H NMR of **3ia**



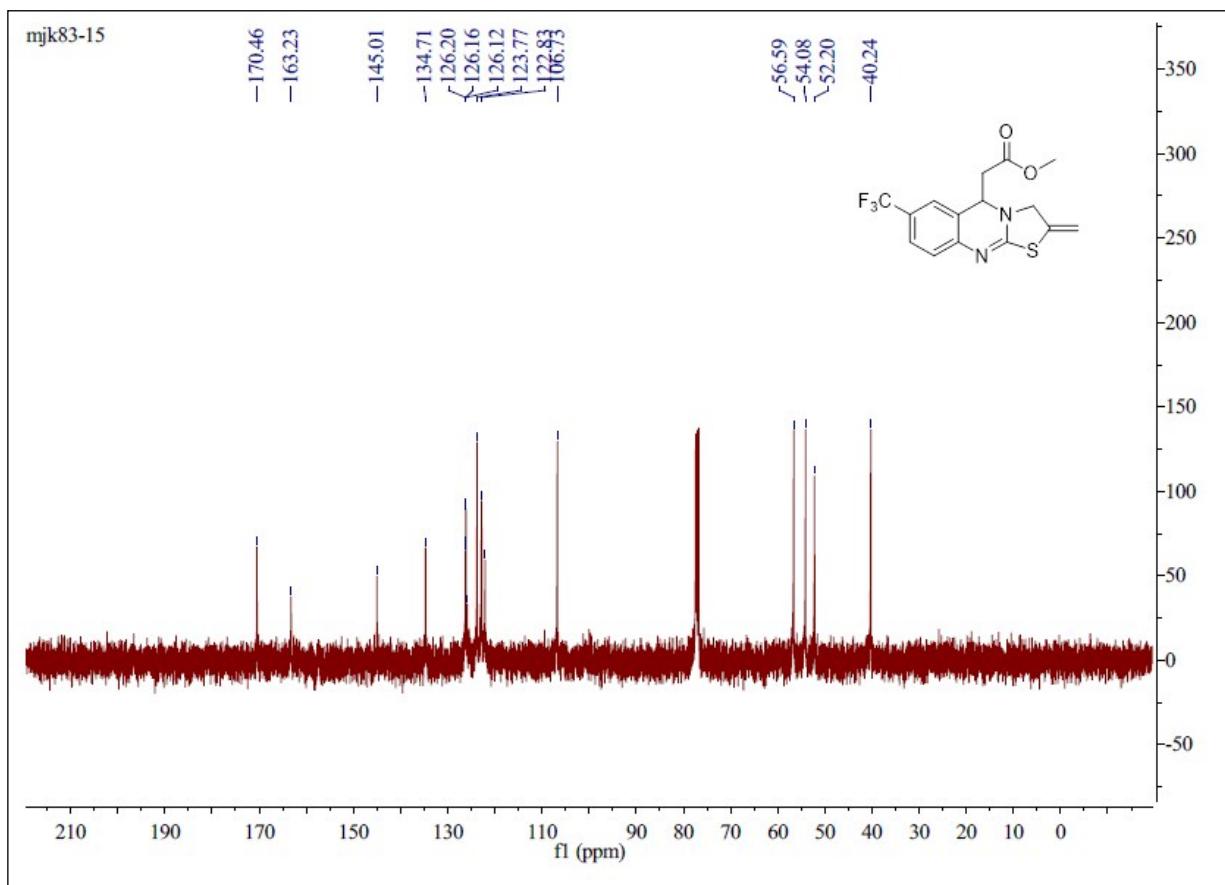
^{13}C NMR of **3ia**



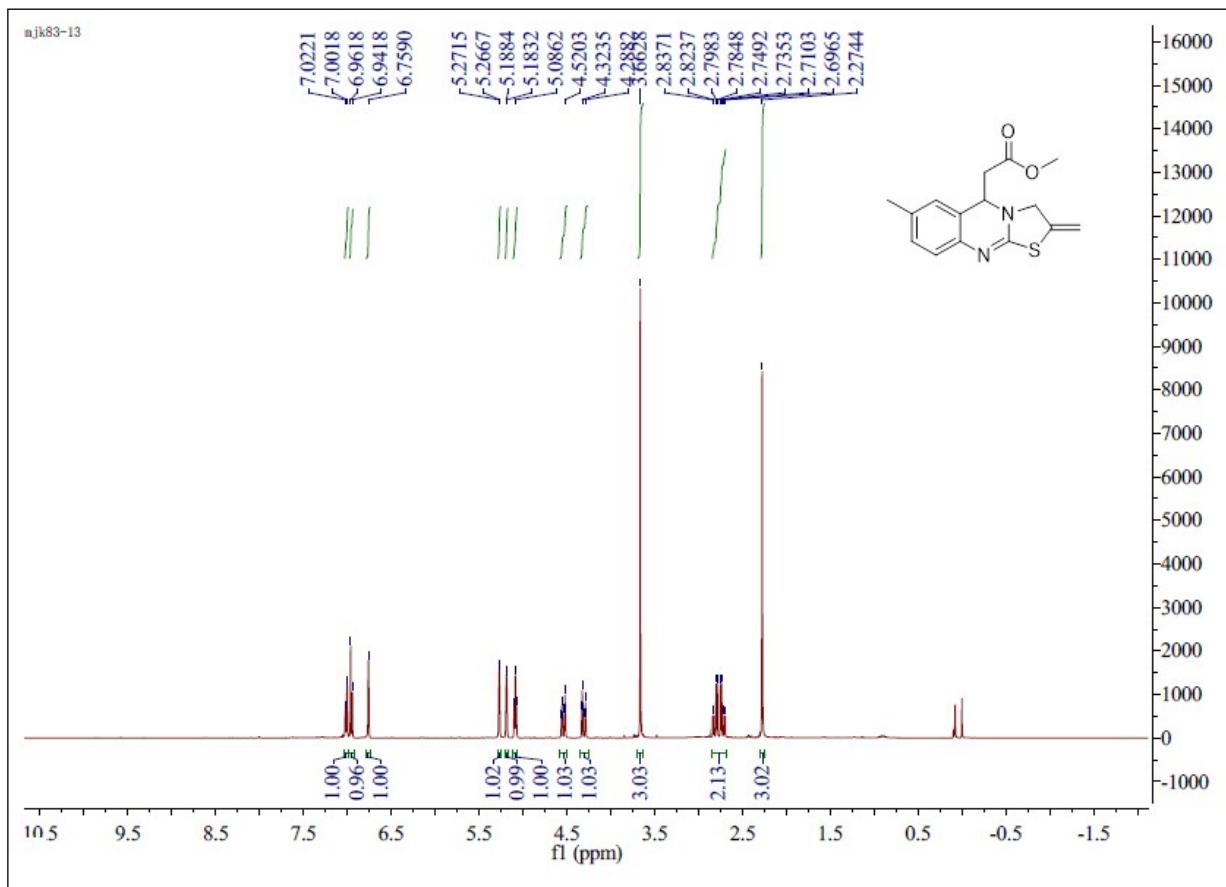
^1H NMR of **3ja**



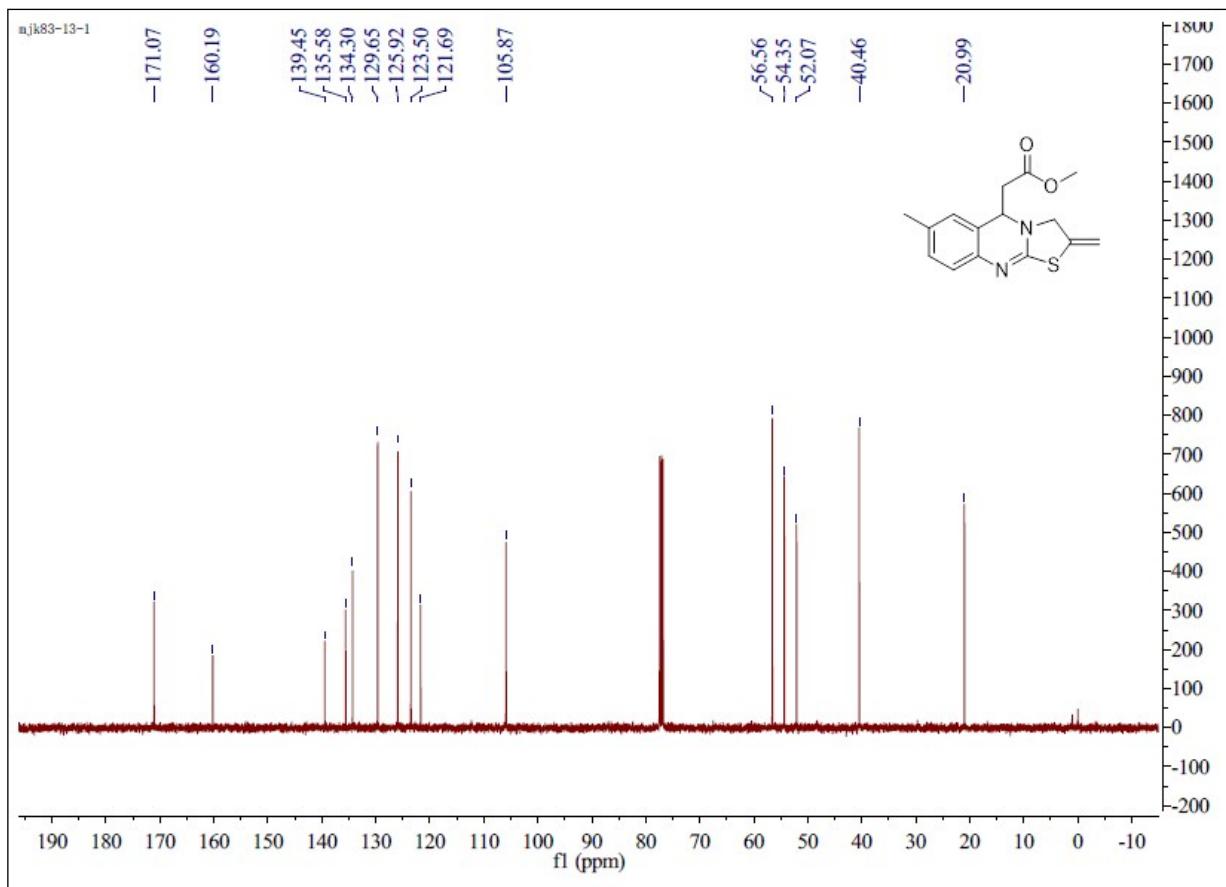
¹³C NMR of 3ja



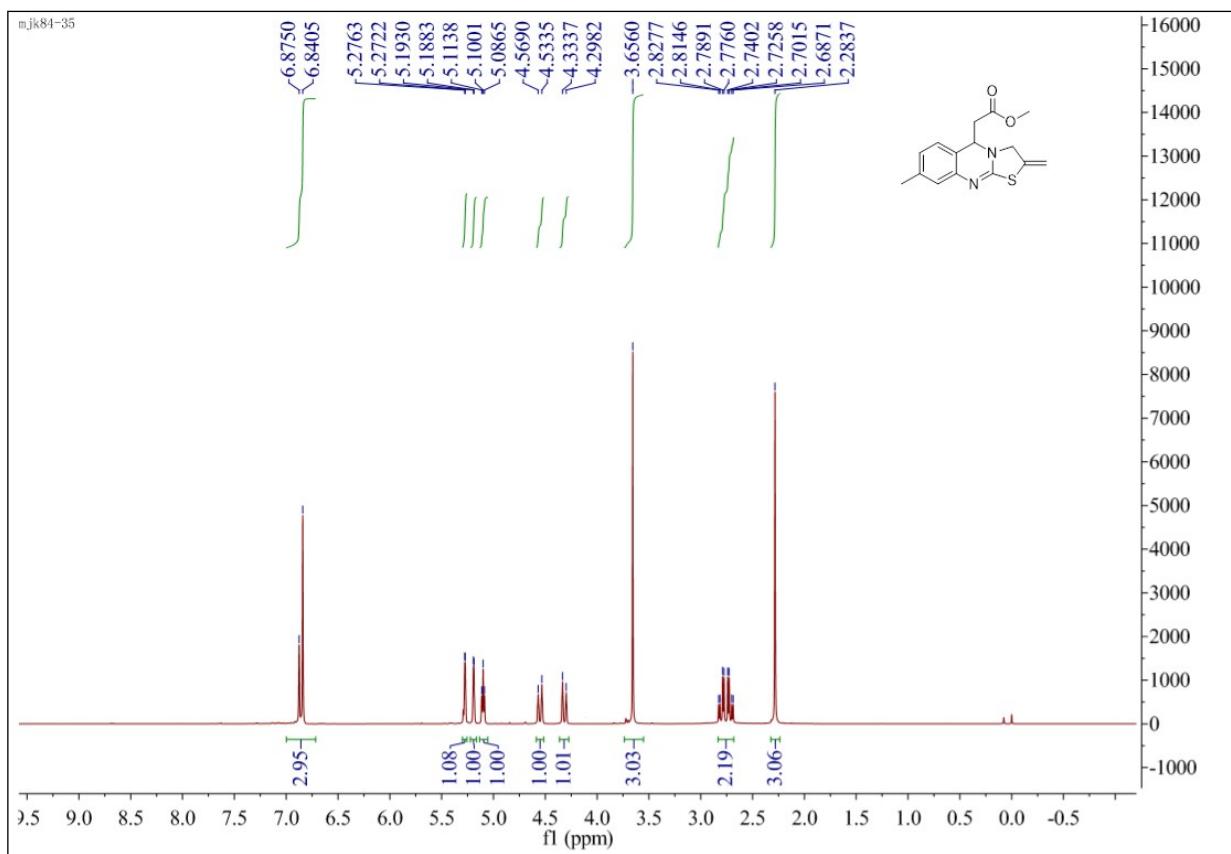
¹H NMR of 3ka



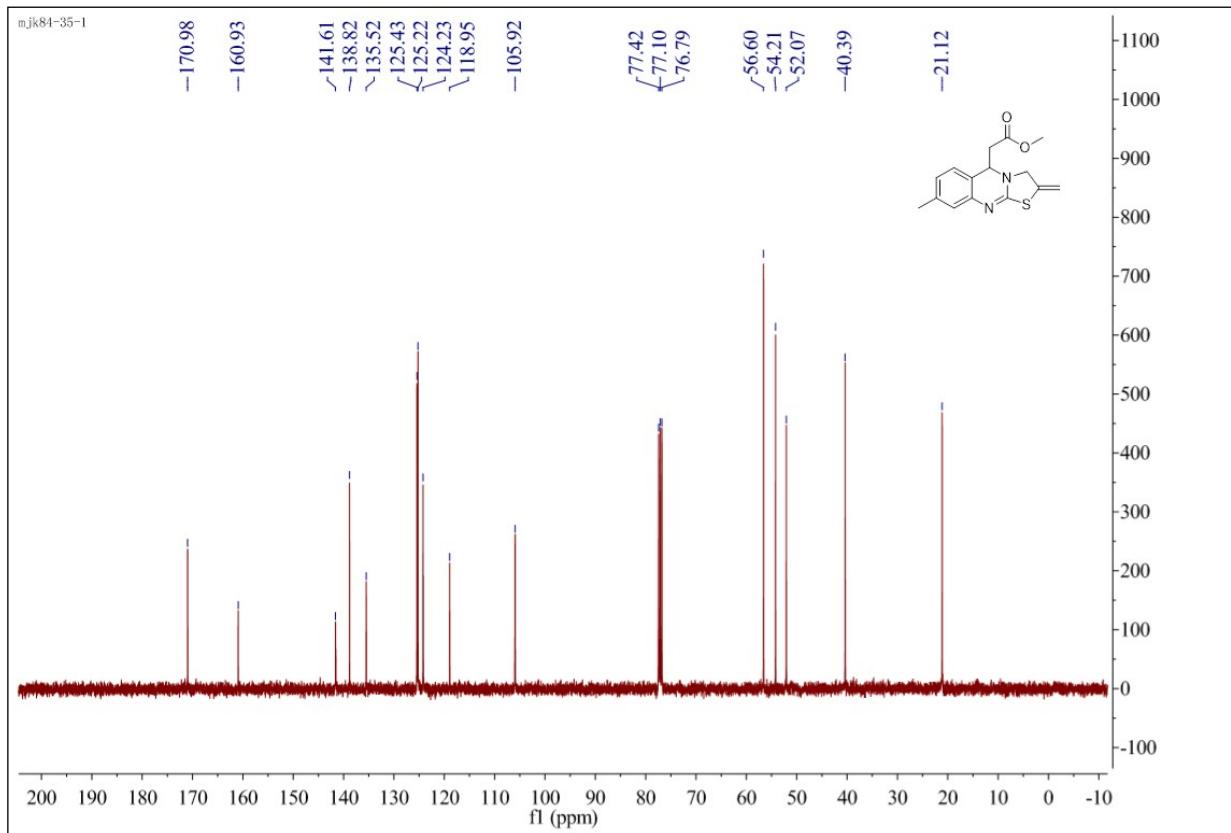
¹³C NMR of 3ka



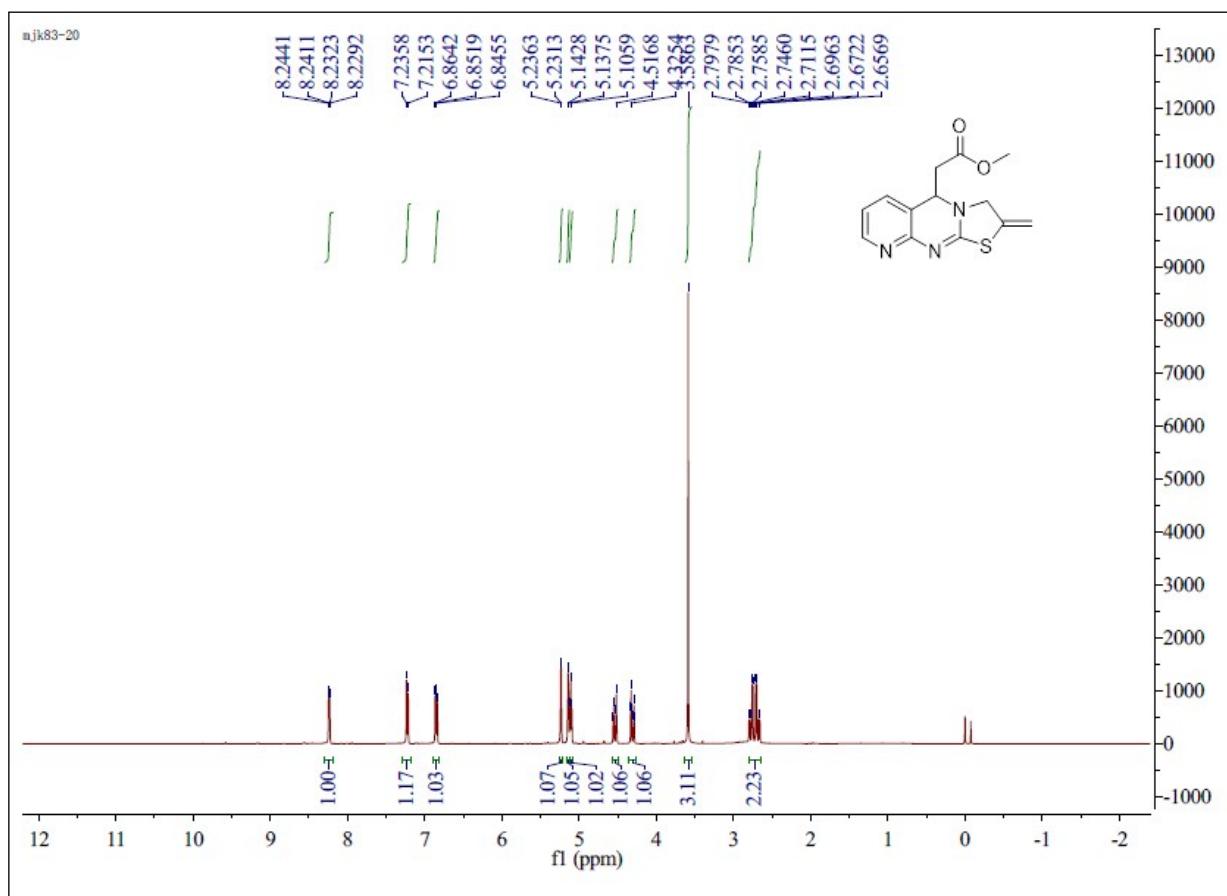
¹H NMR of 3la



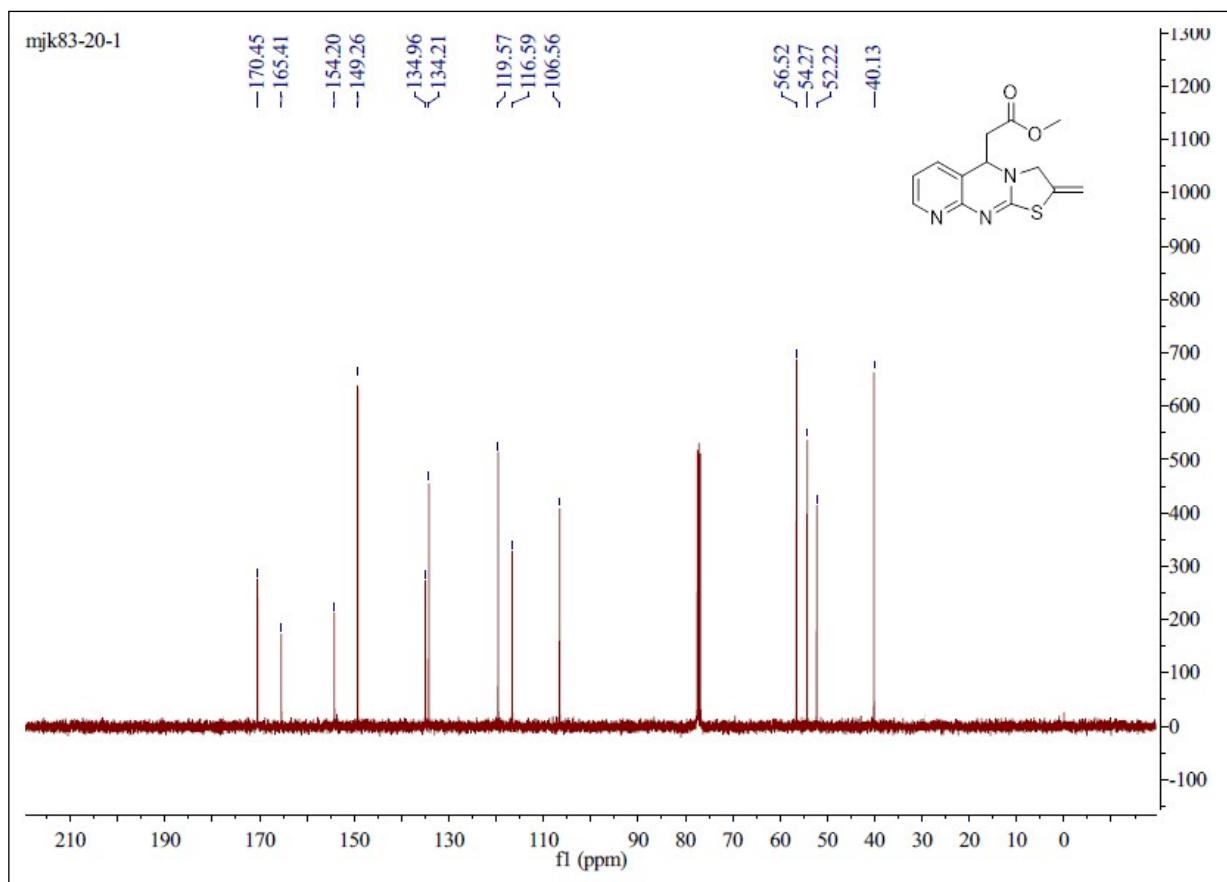
¹³C NMR of 3la



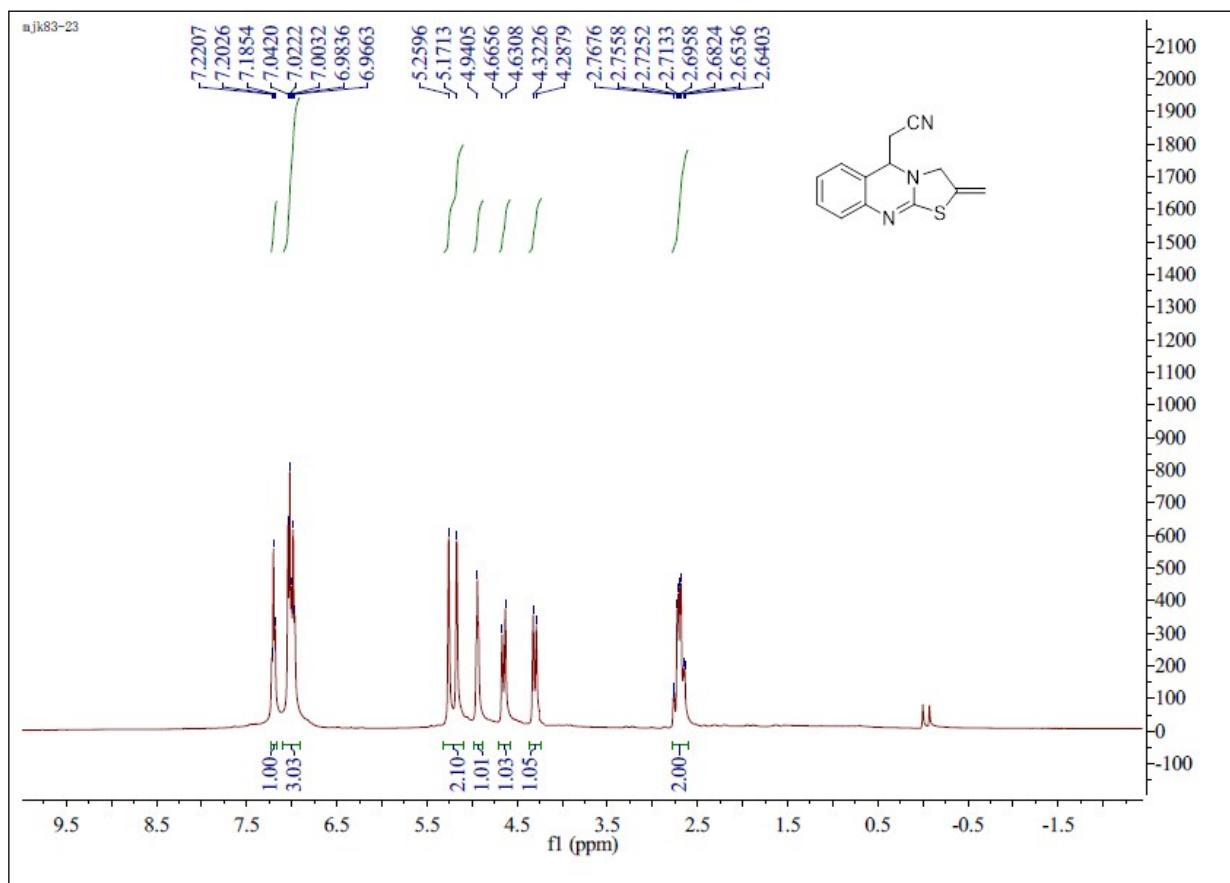
¹H NMR of 3ma



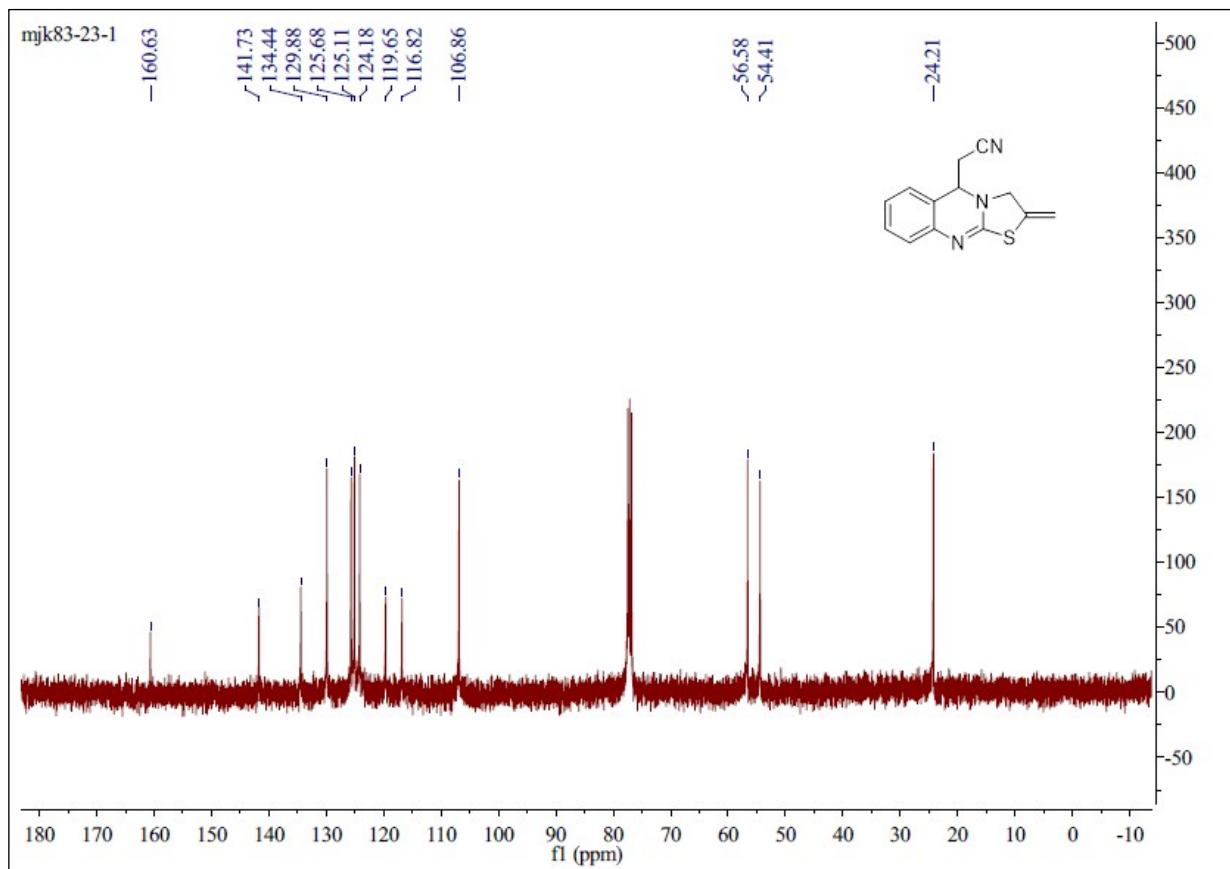
¹³C NMR of 3ma



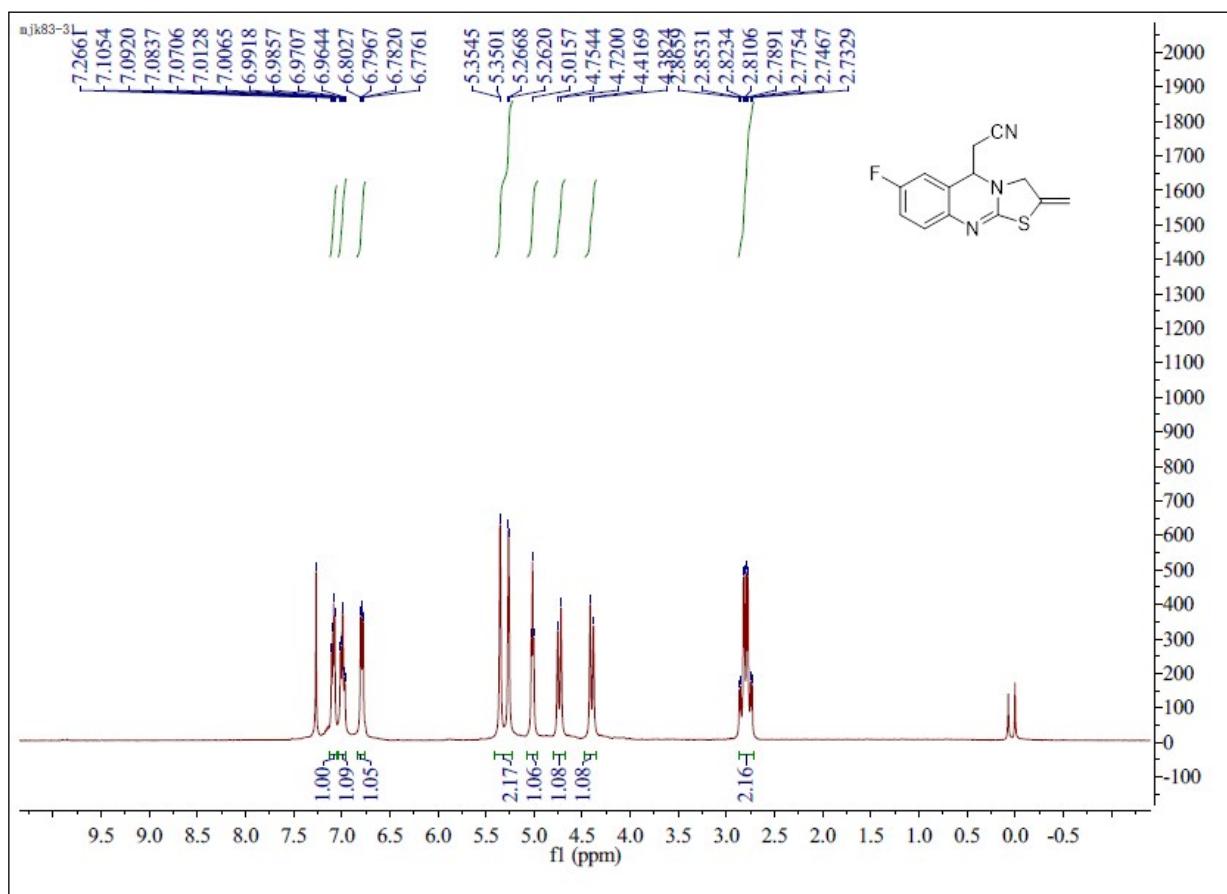
¹H NMR of 3na



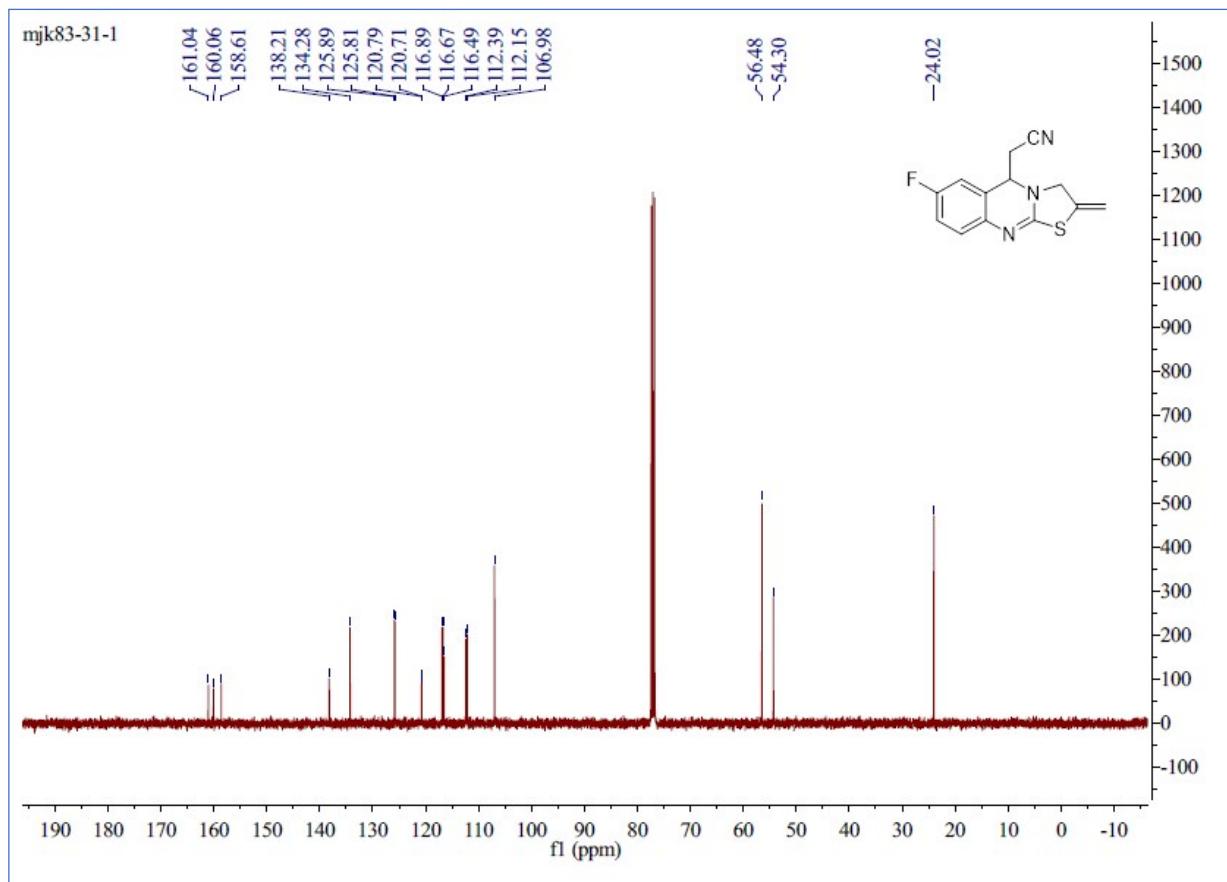
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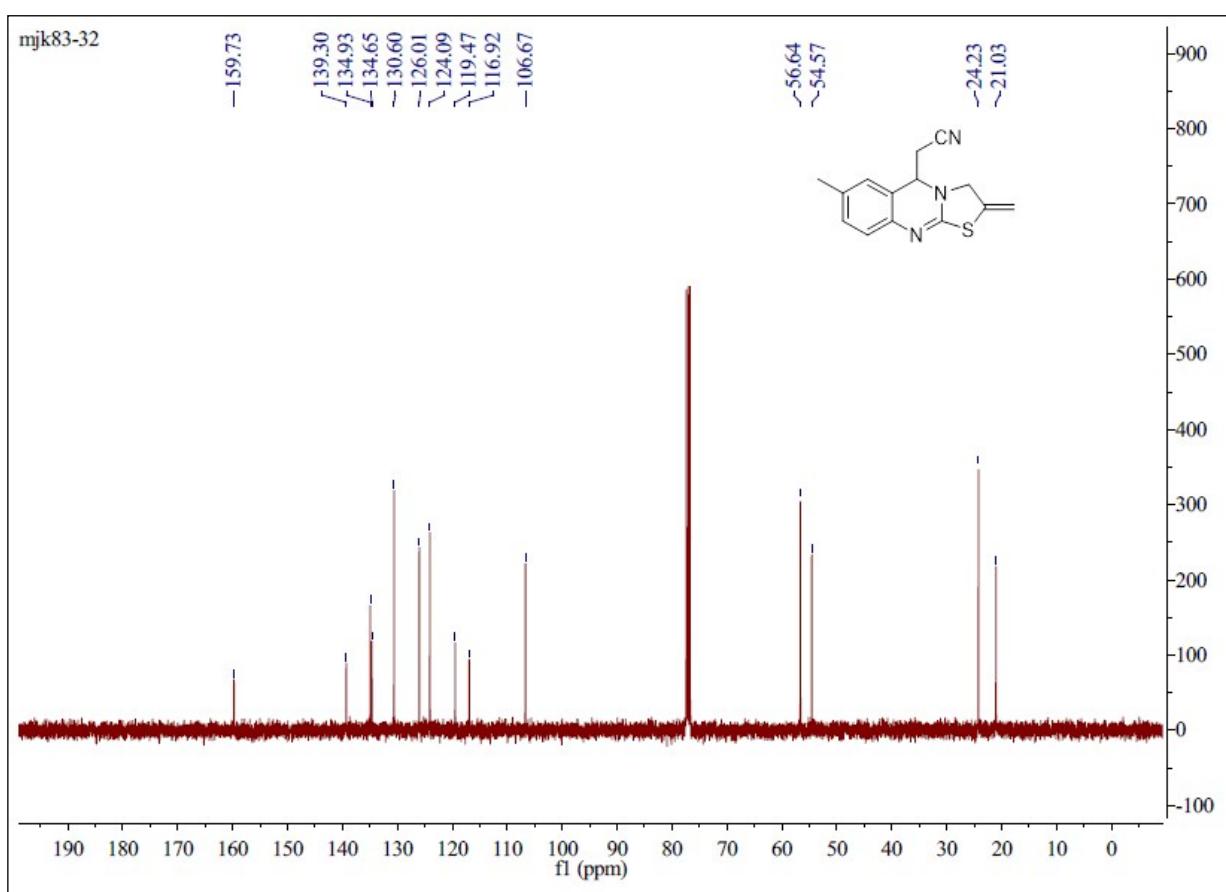
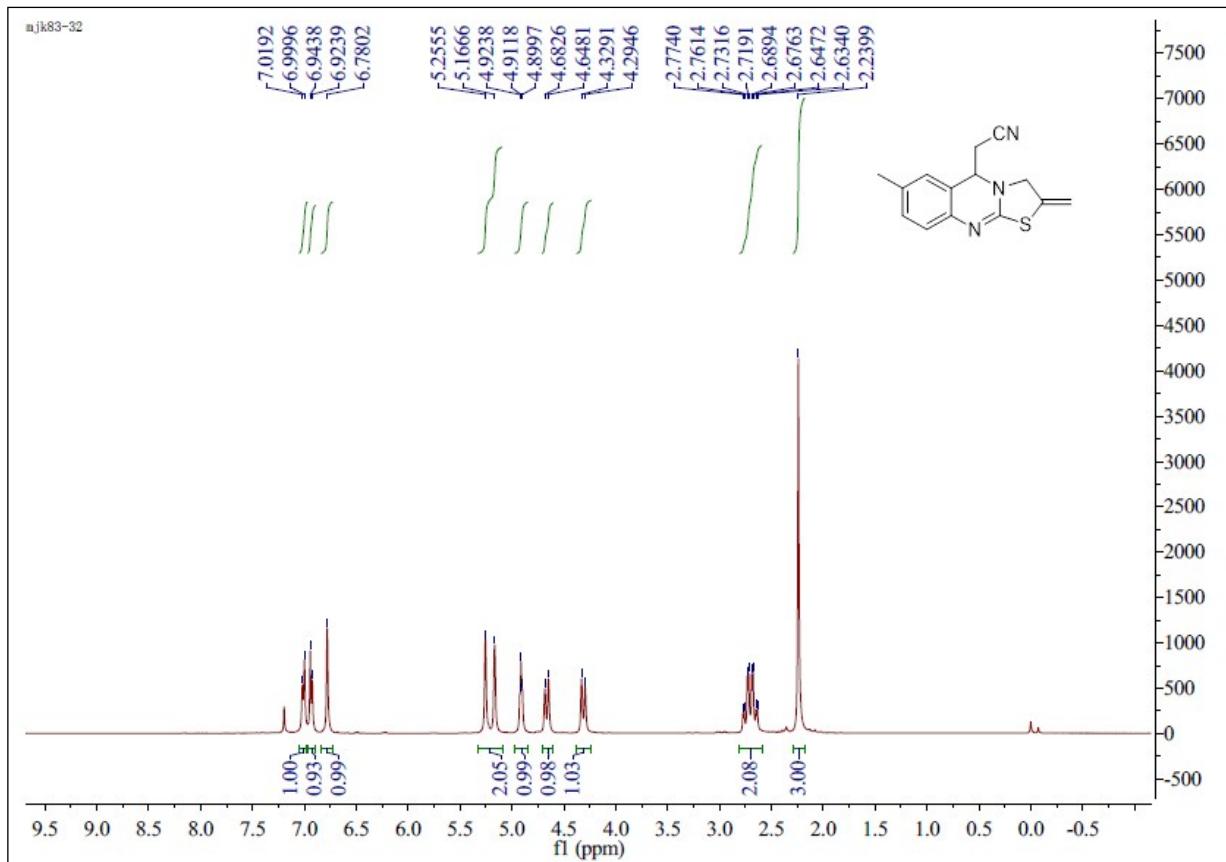
¹H NMR of 3oa



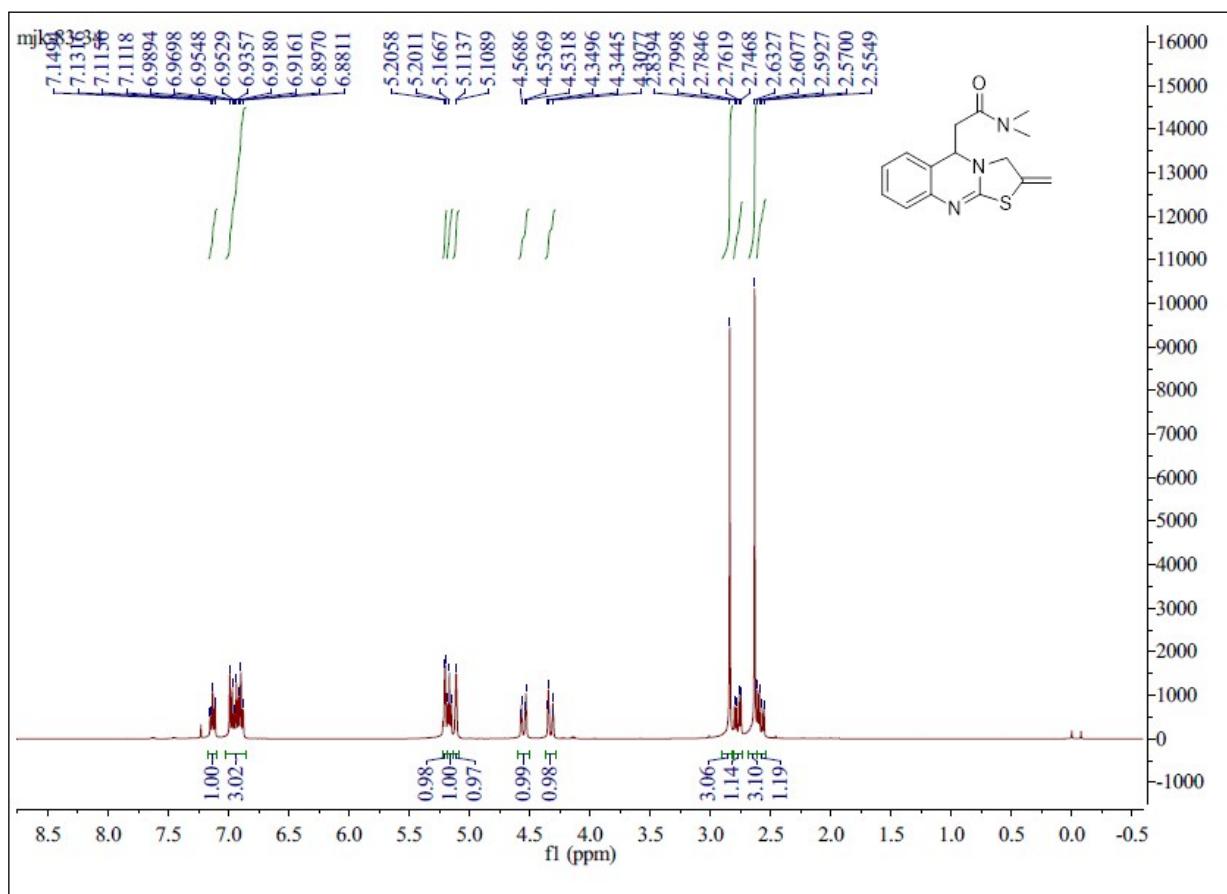
¹³C NMR of 3oa



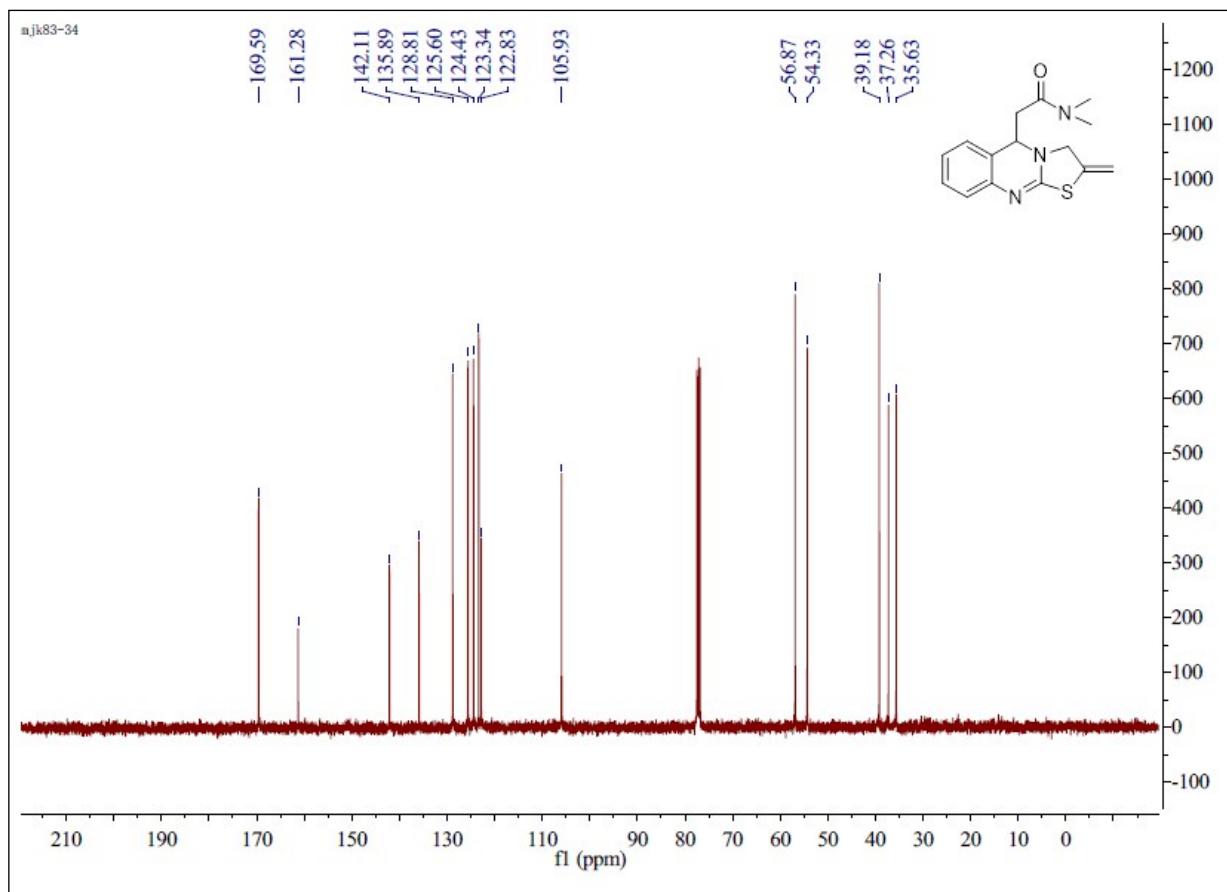
¹H NMR of 3pa



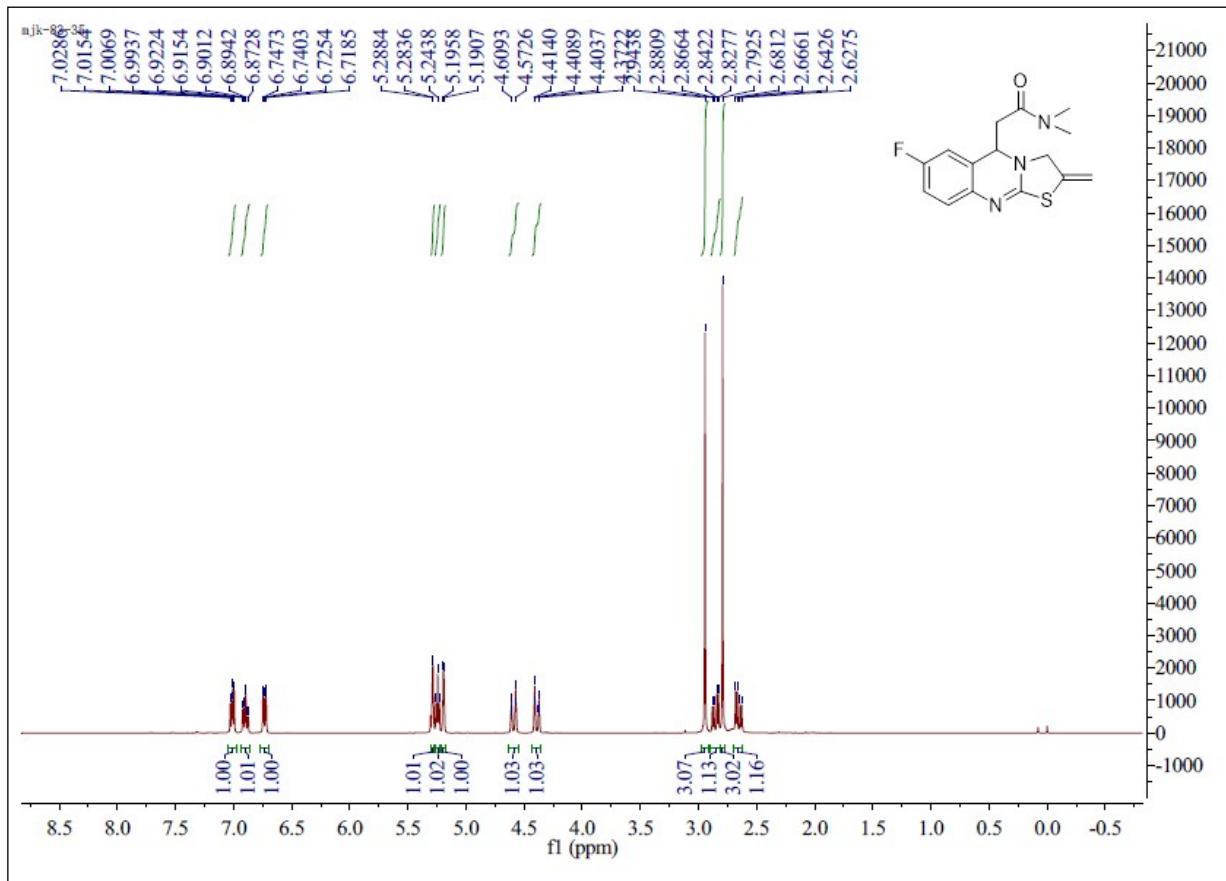
¹H NMR of 3qa



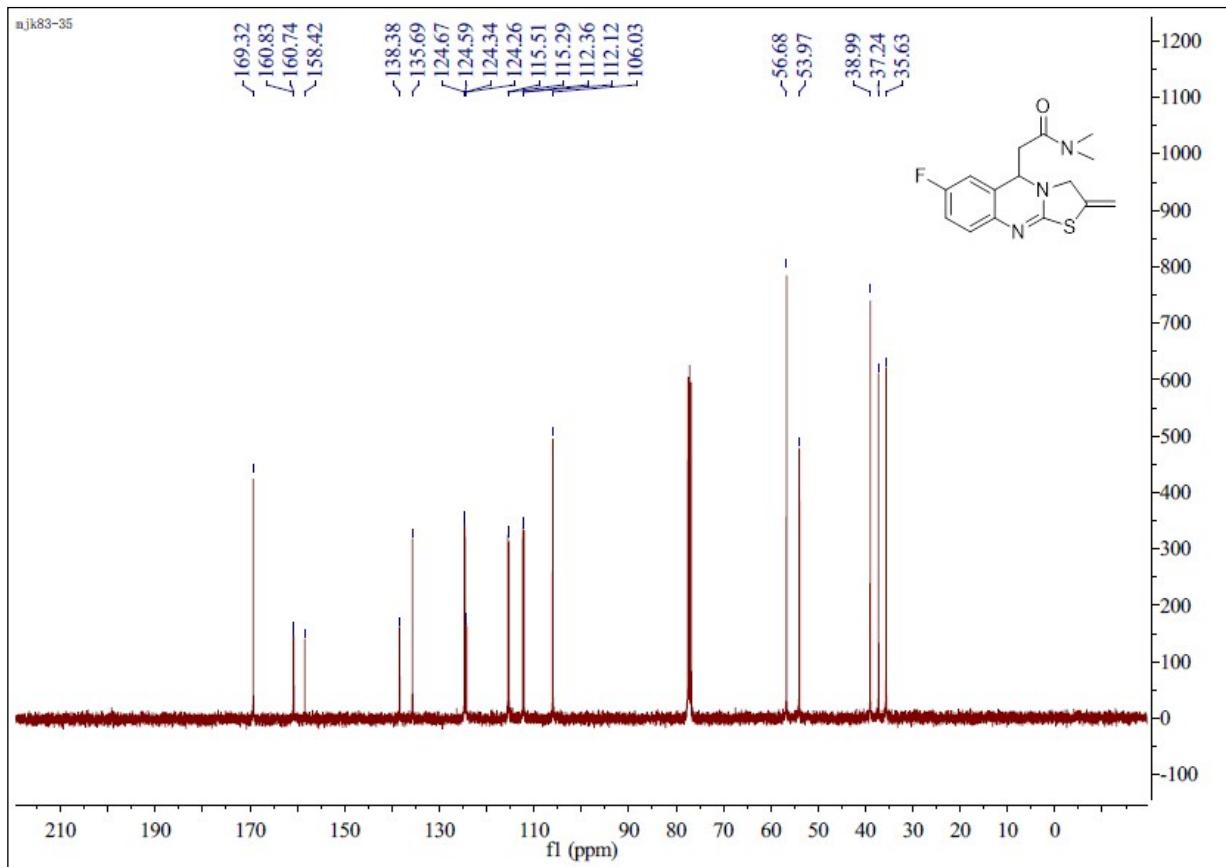
¹³C NMR of 3qa



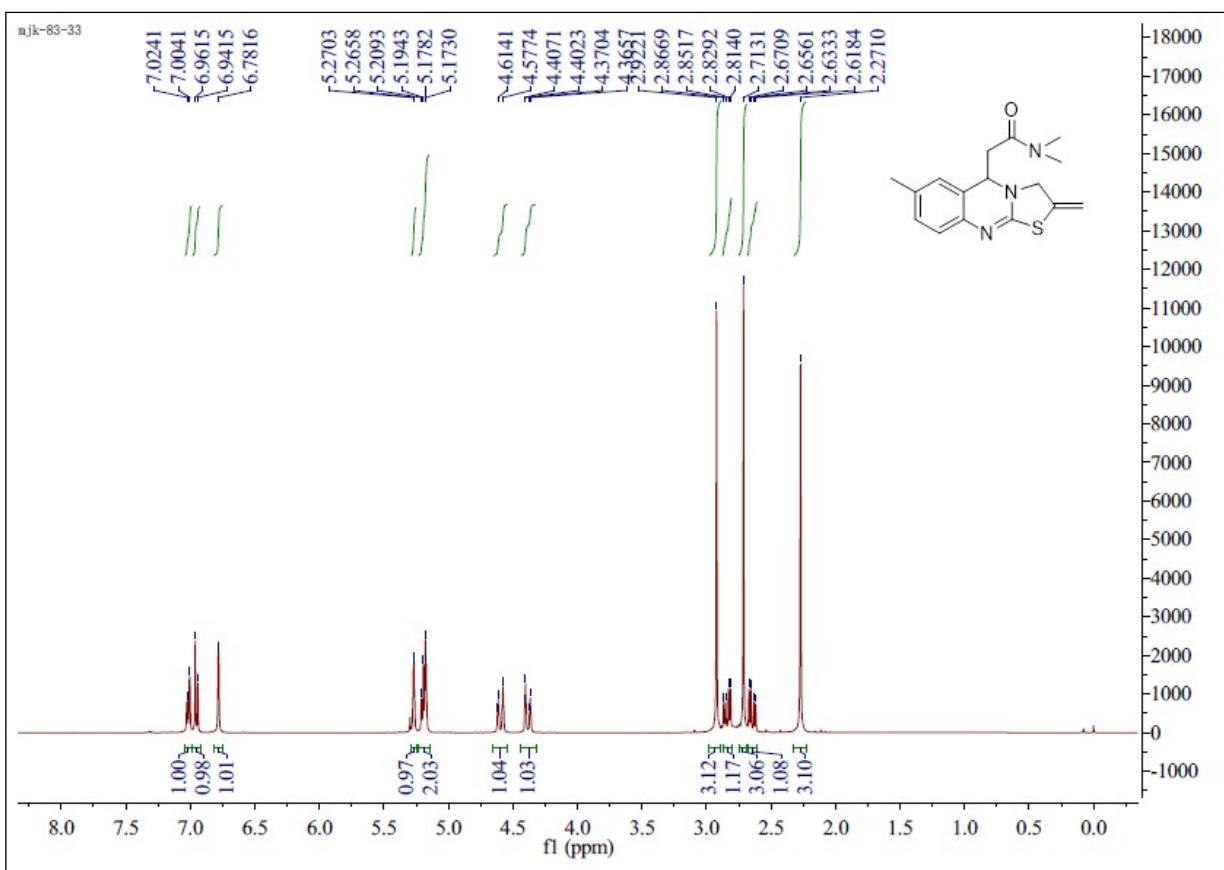
¹H NMR of 3ra



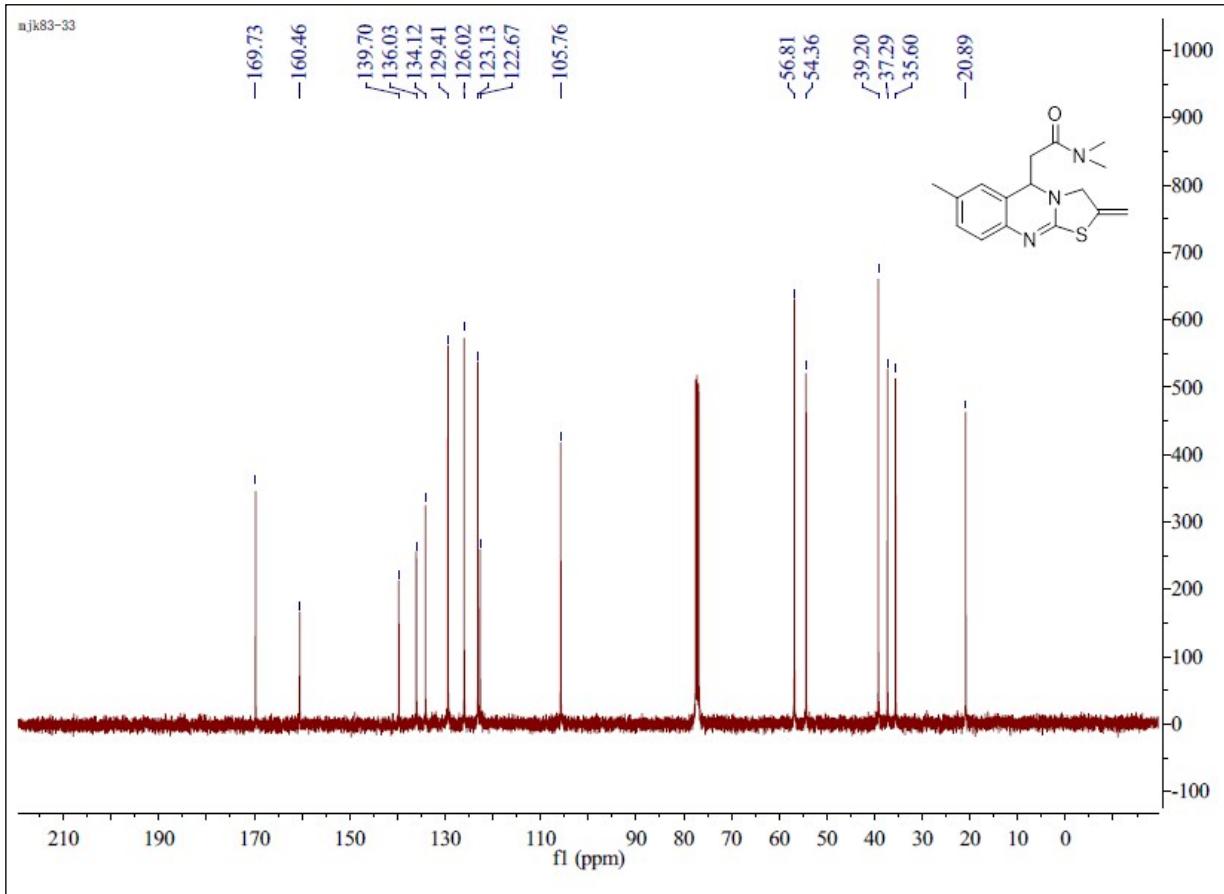
¹³C NMR of 3ra



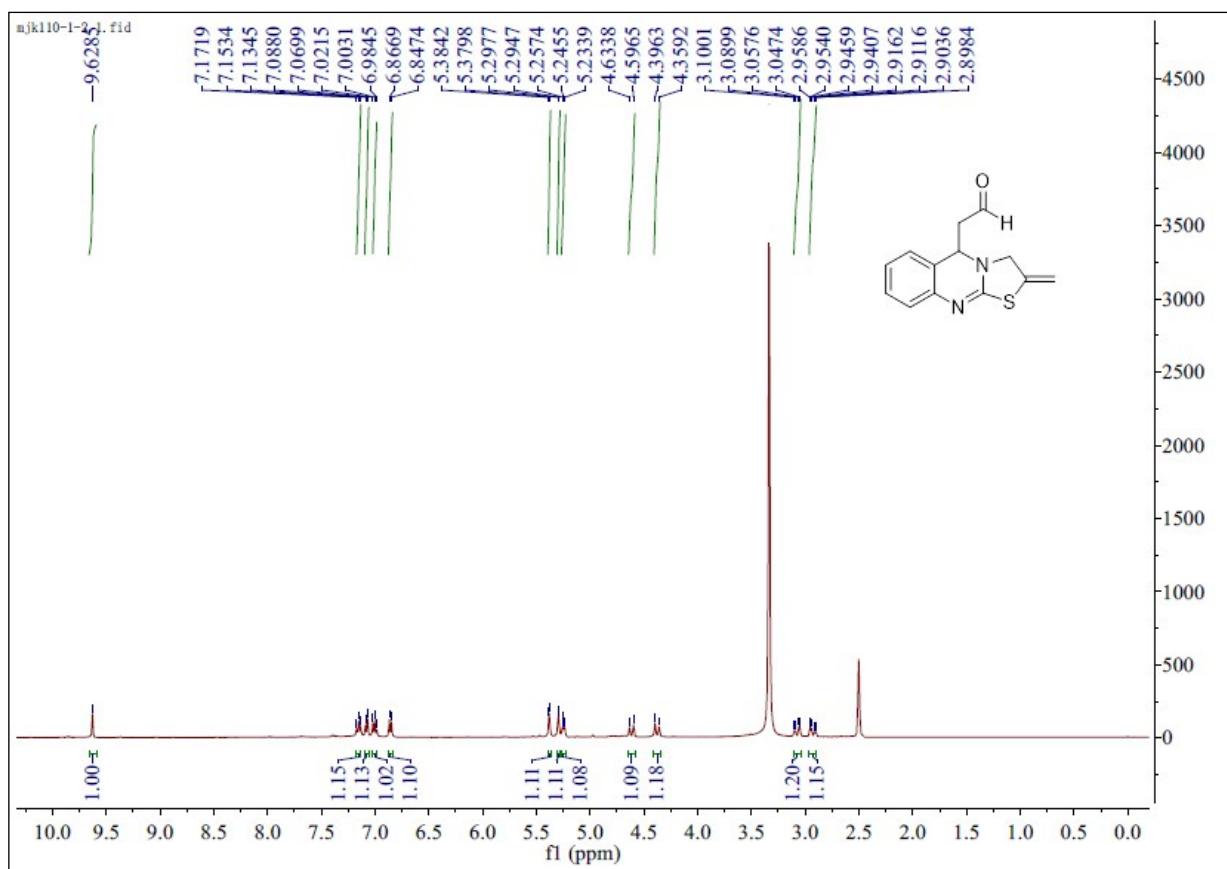
¹H NMR of 3sa



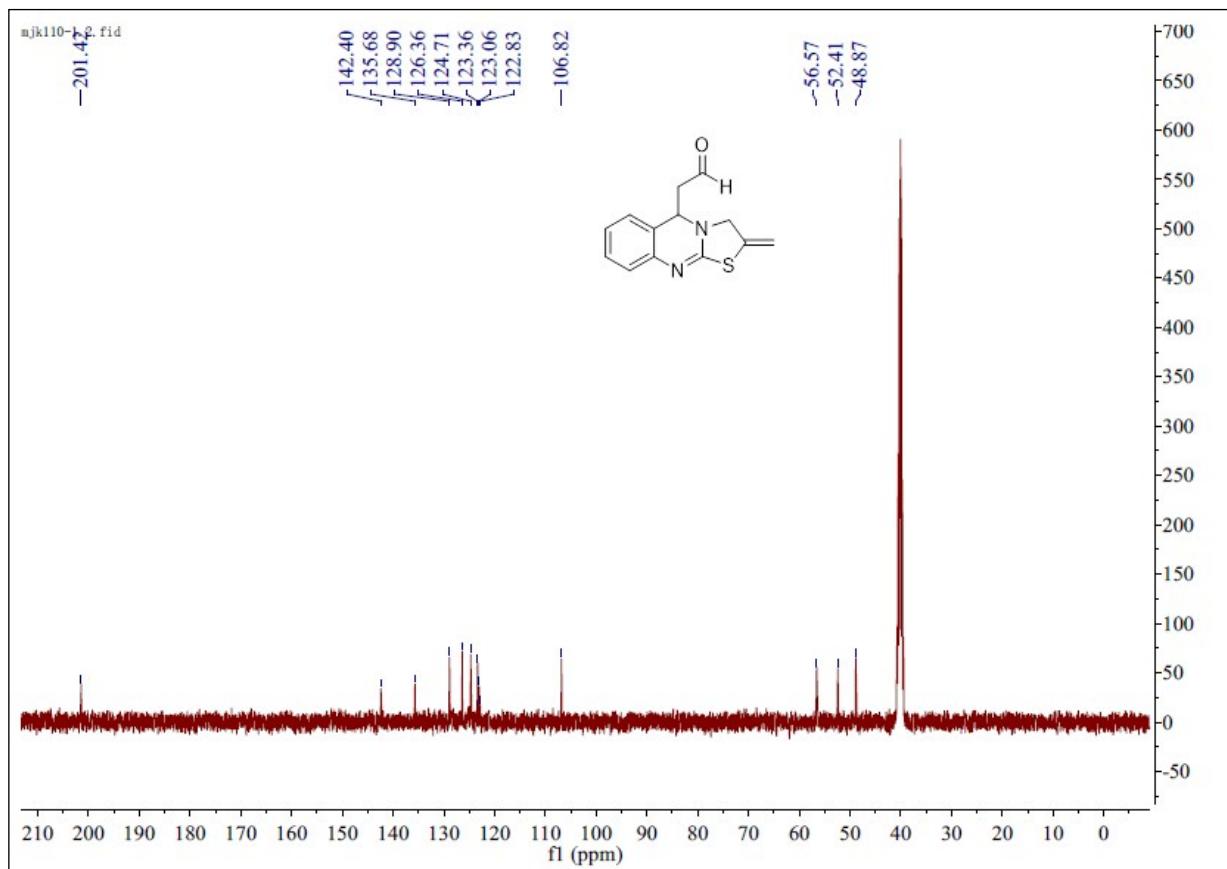
¹³C NMR of 3sa



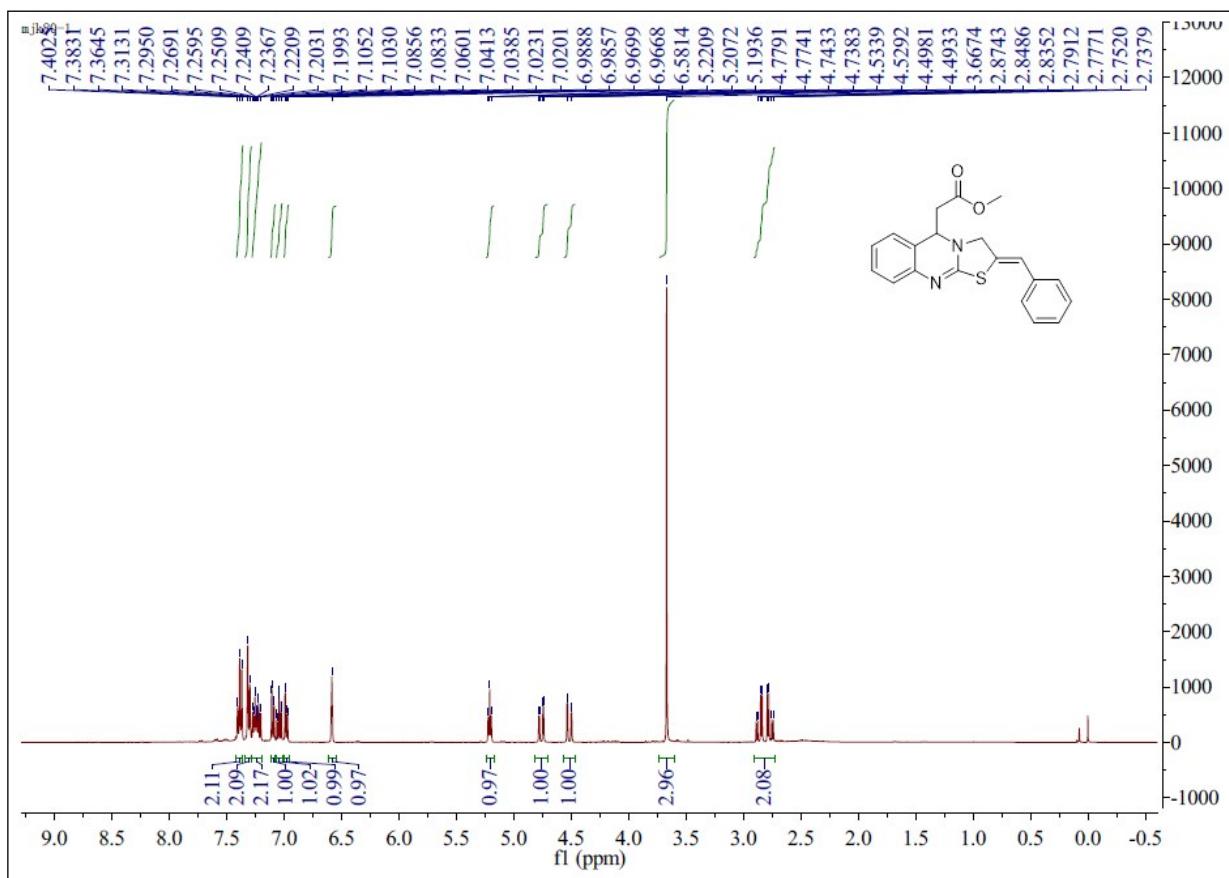
¹H NMR of 3ta



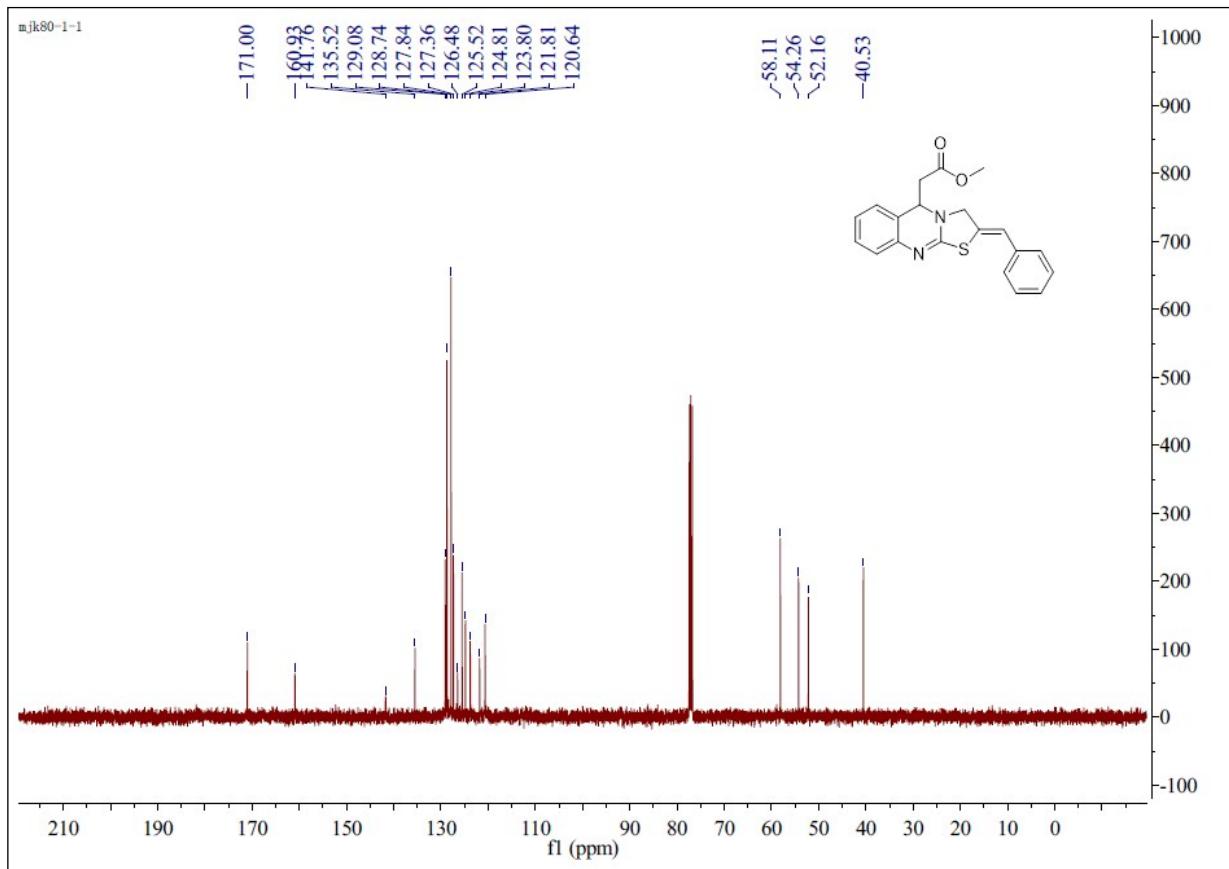
¹³C NMR of 3ta



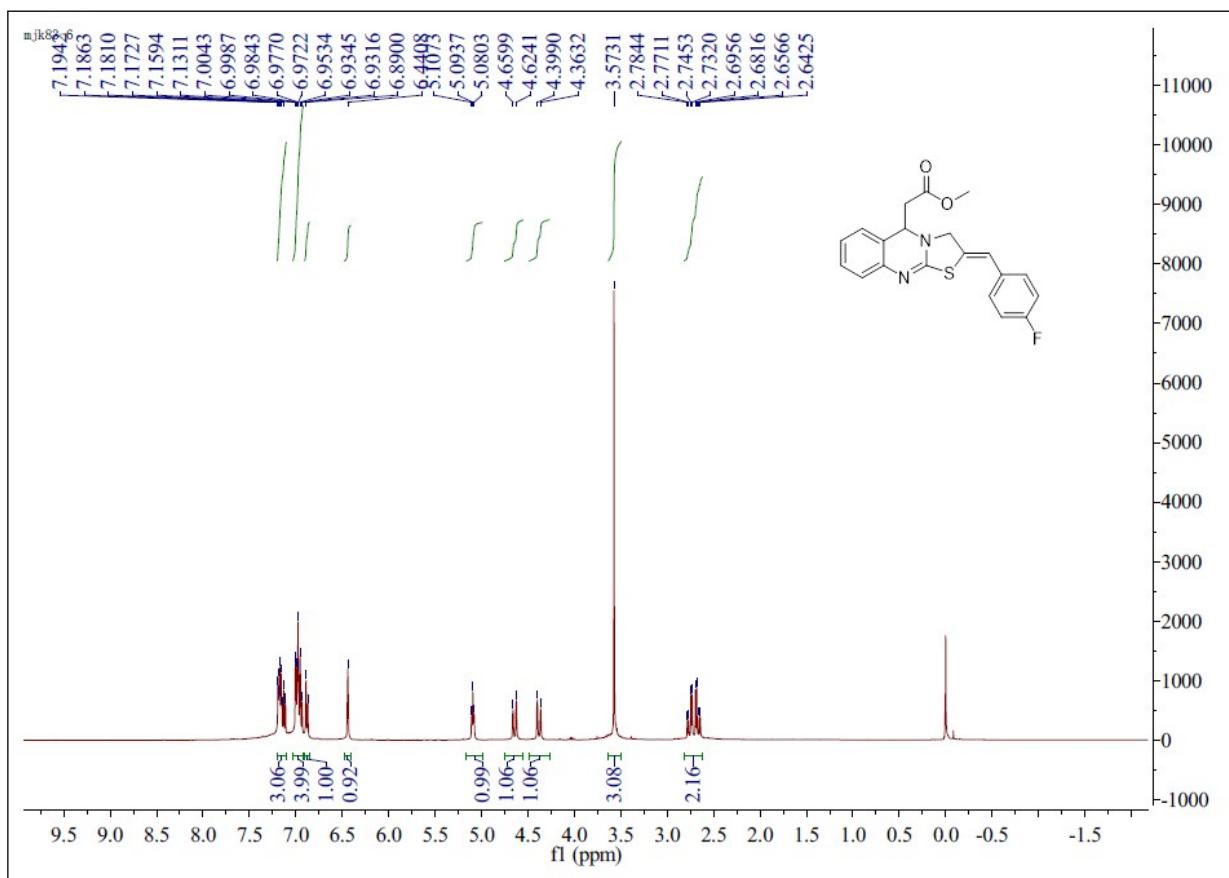
¹H NMR of 3ab



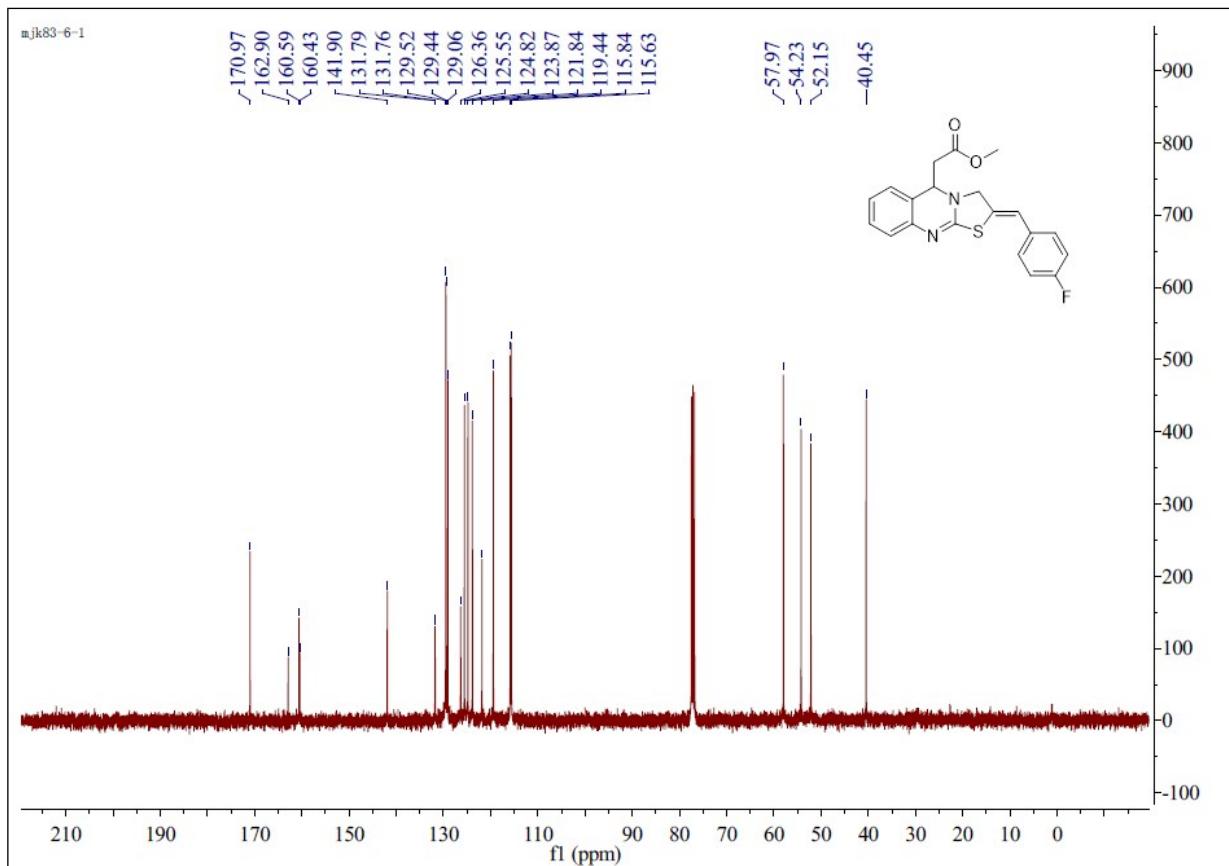
¹H NMR of 3ab



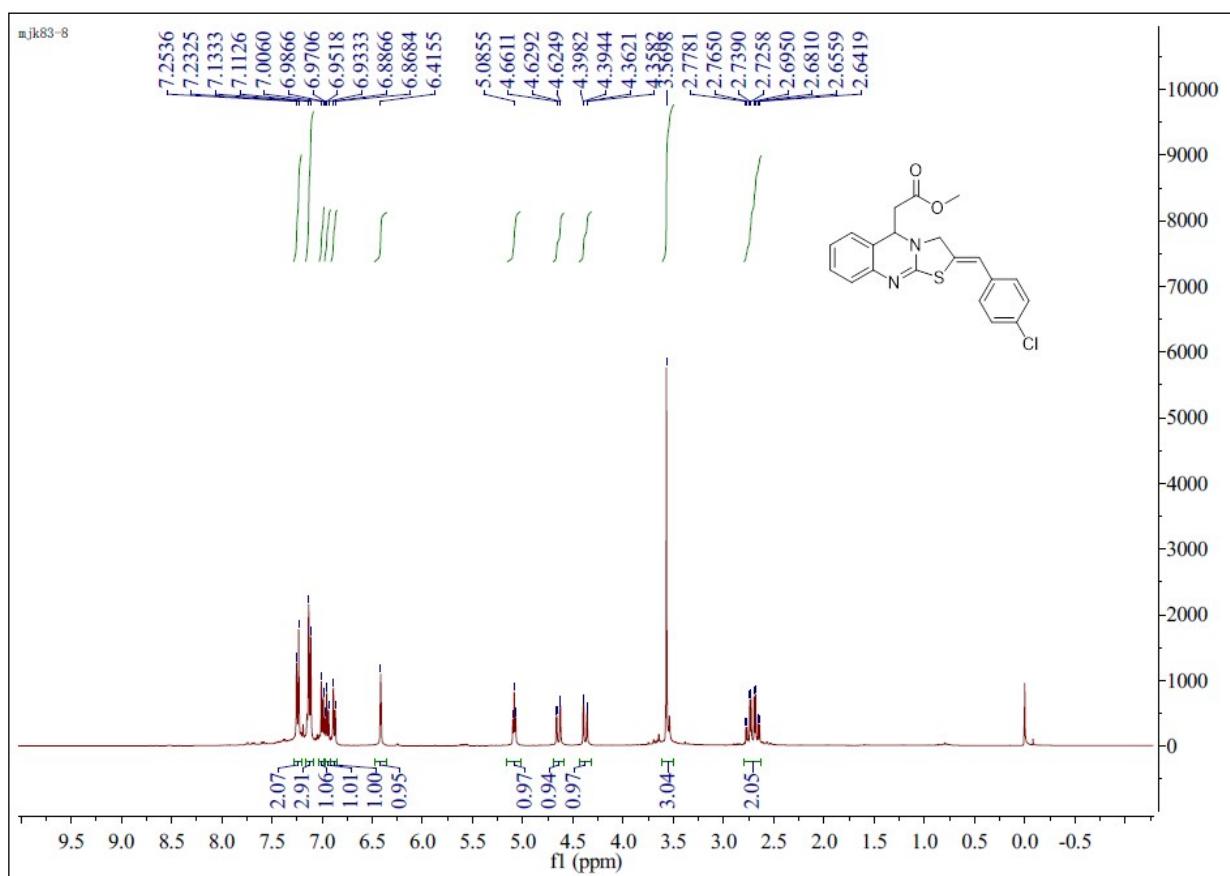
¹H NMR of 3ac



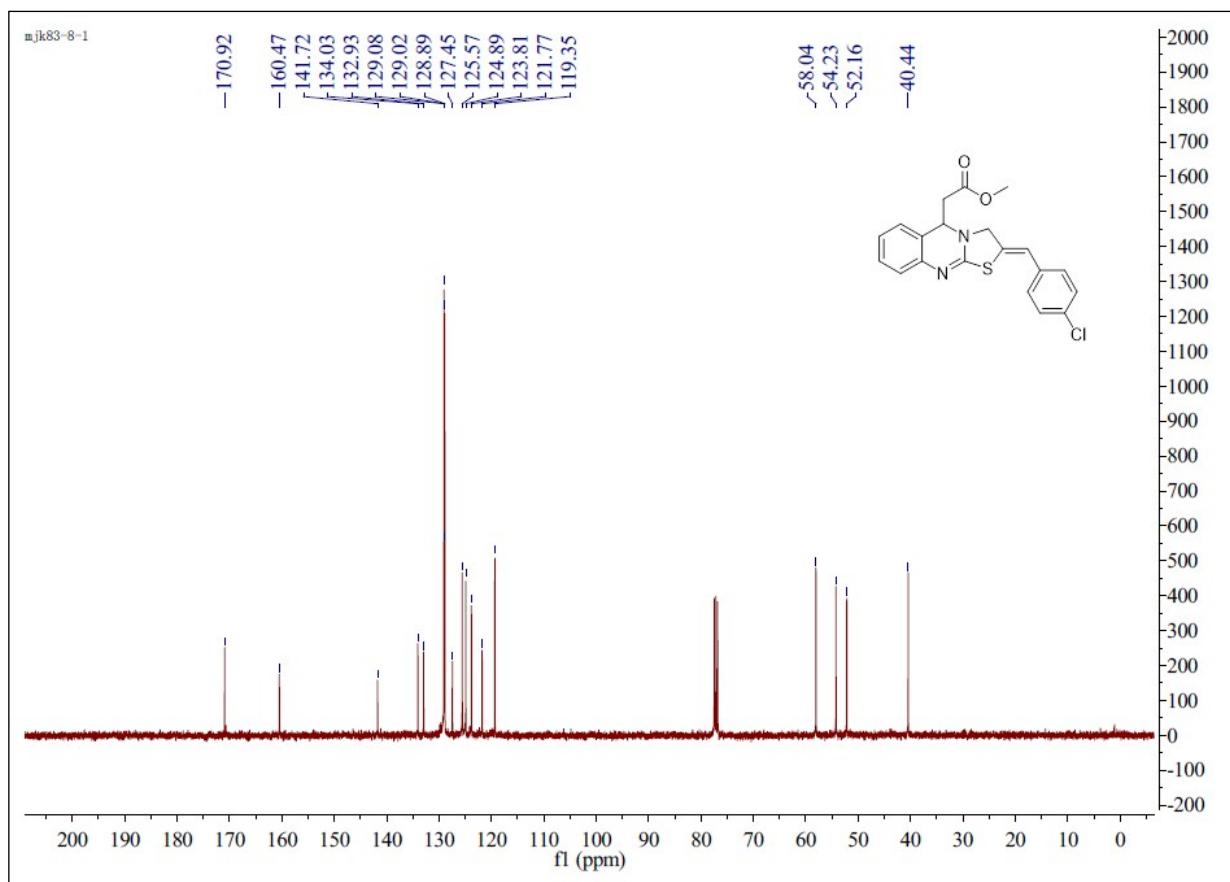
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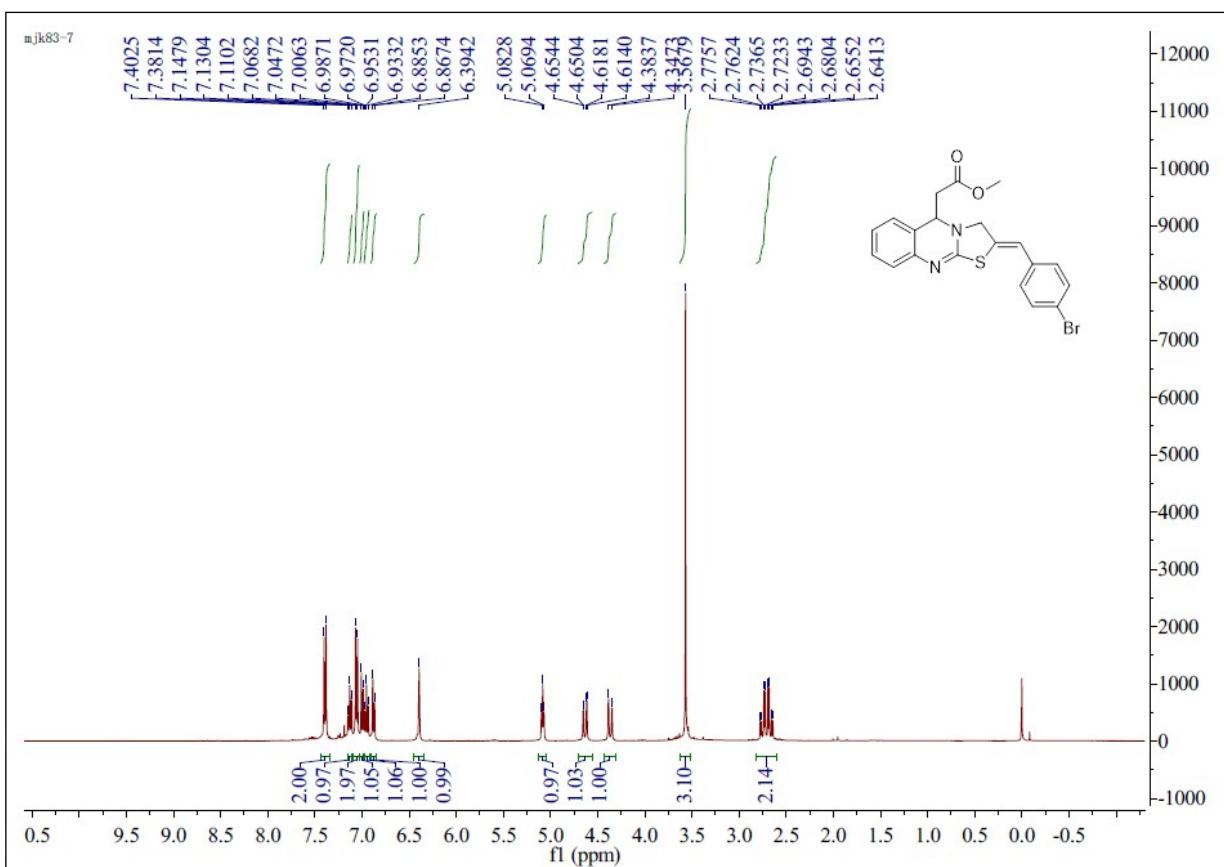
¹H NMR of 3ad



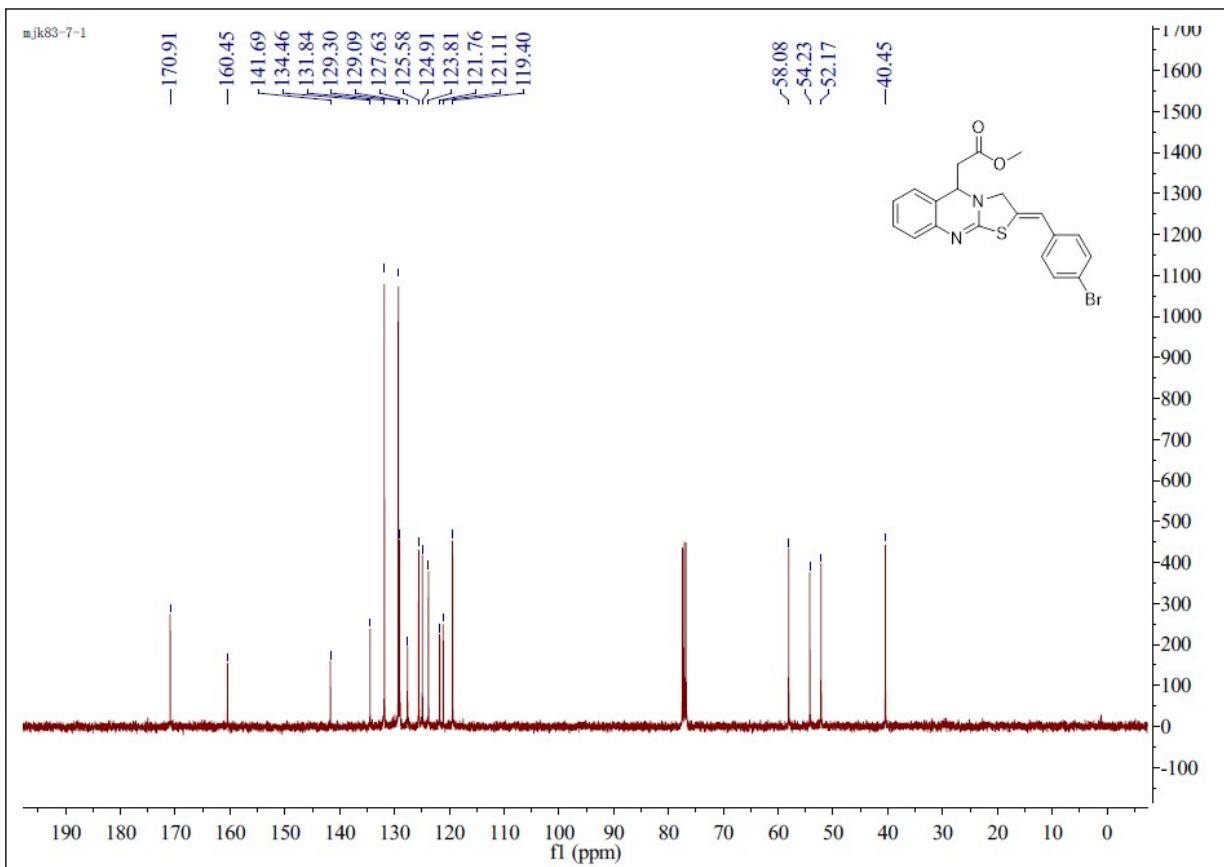
¹³C NMR of 3ad



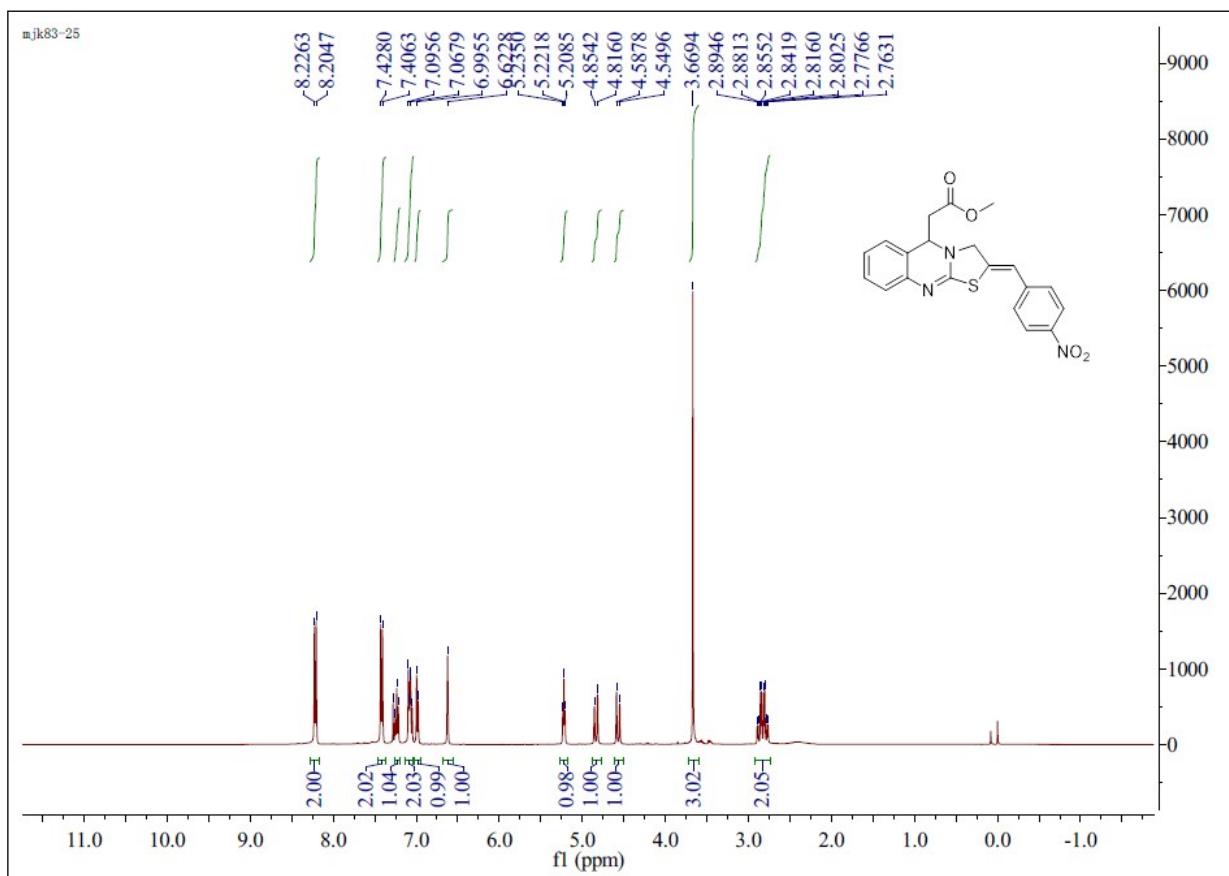
¹H NMR of 3ae



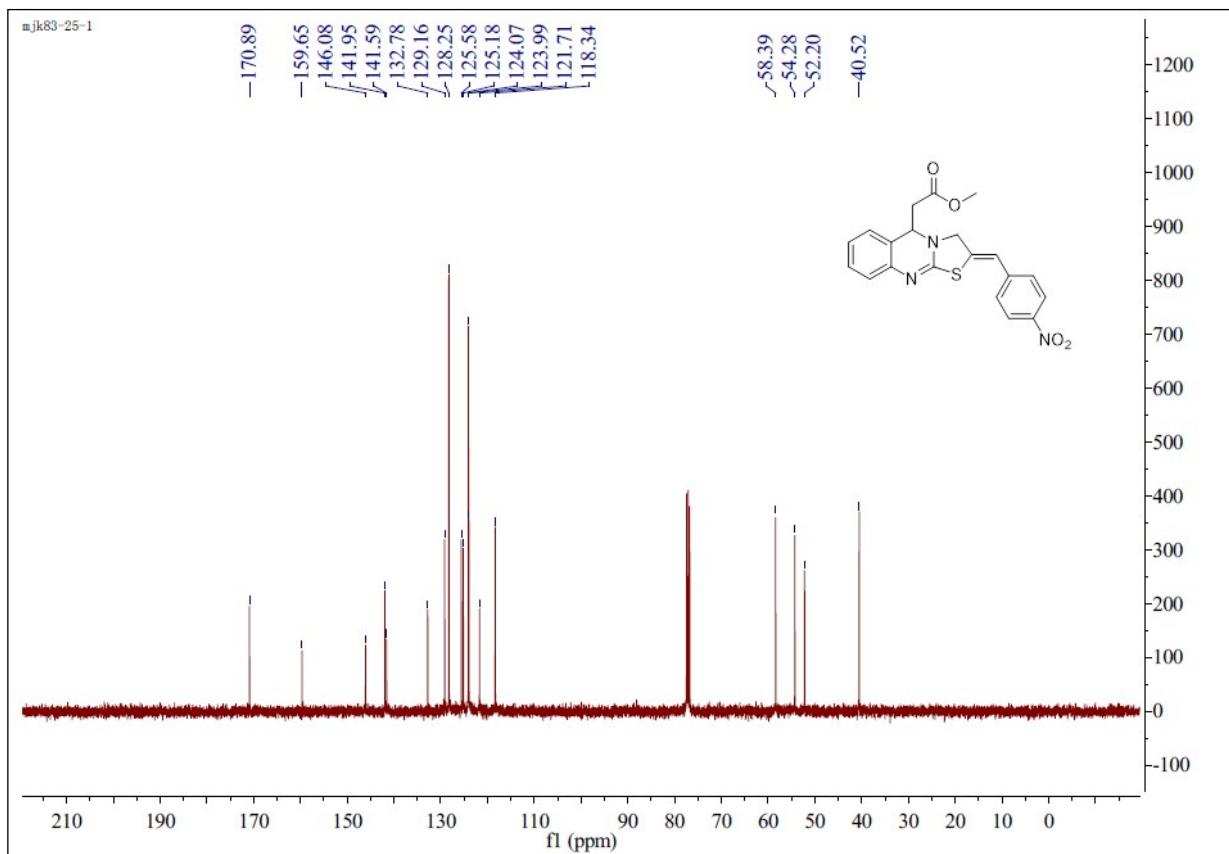
¹³C NMR of 3ae



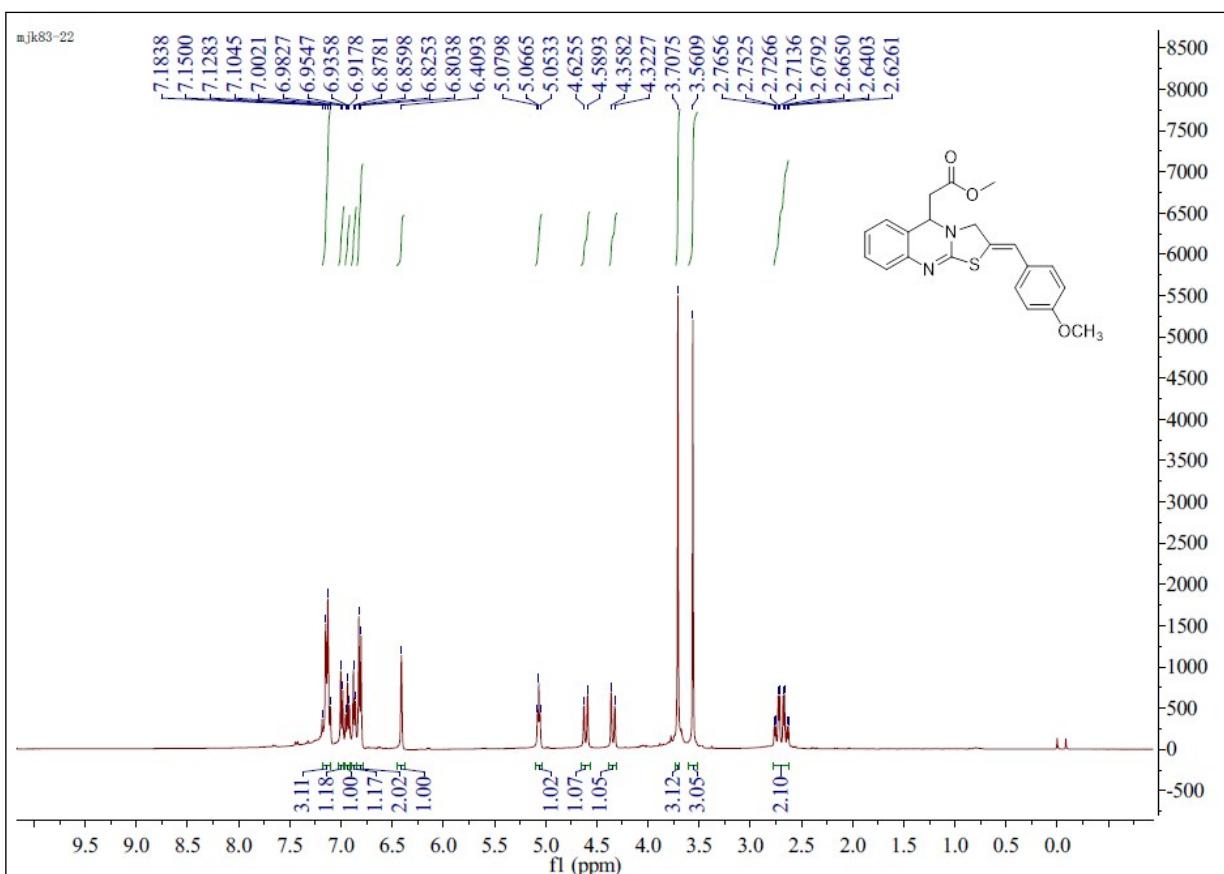
¹H NMR of 3af



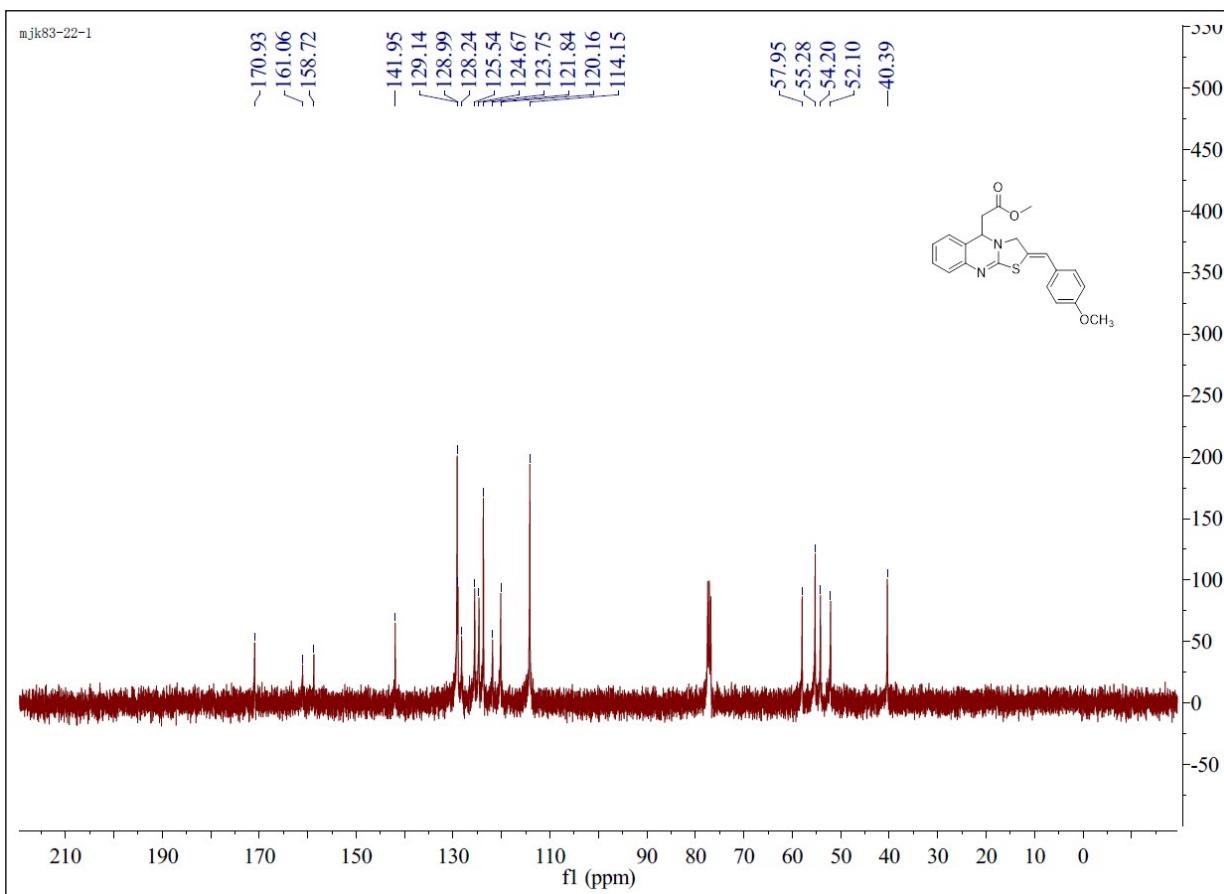
^{13}C NMR of 3af



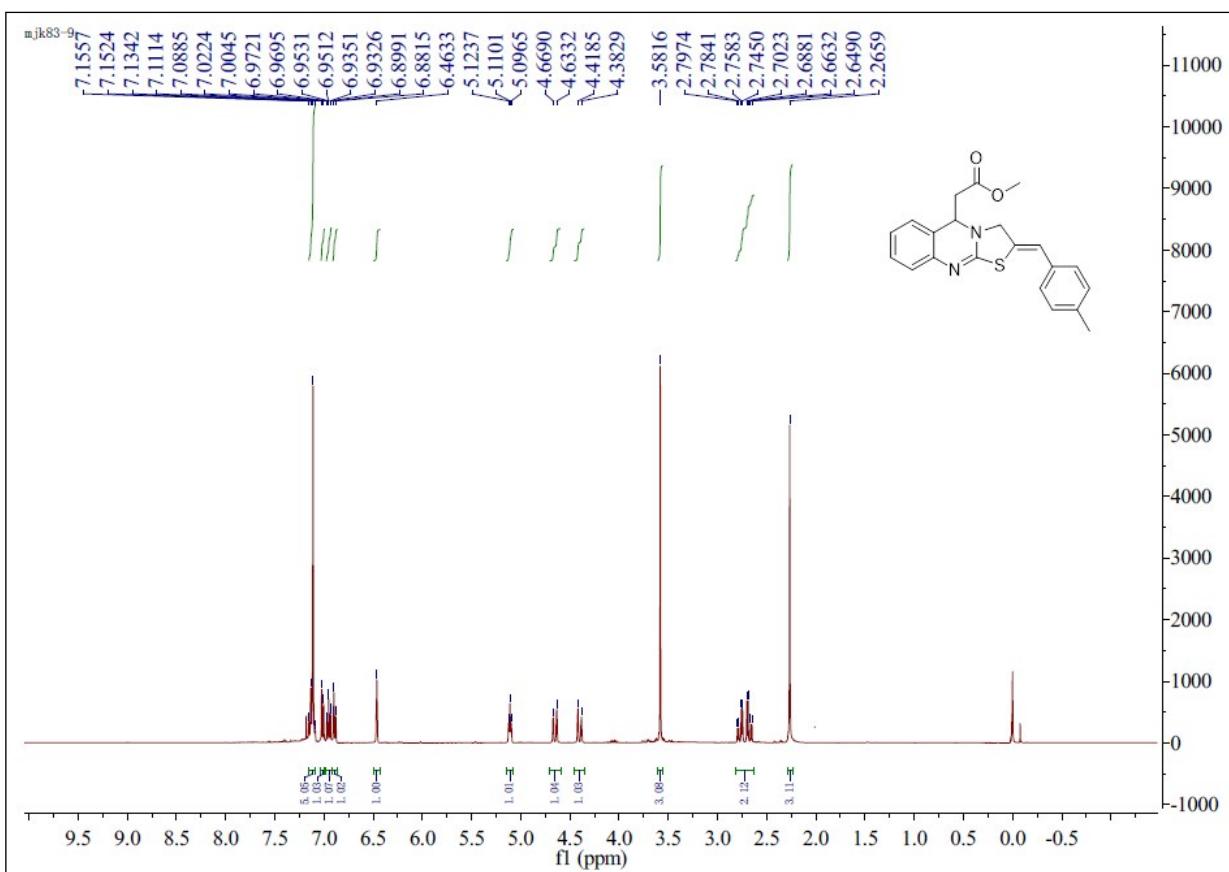
^1H NMR of 3ag



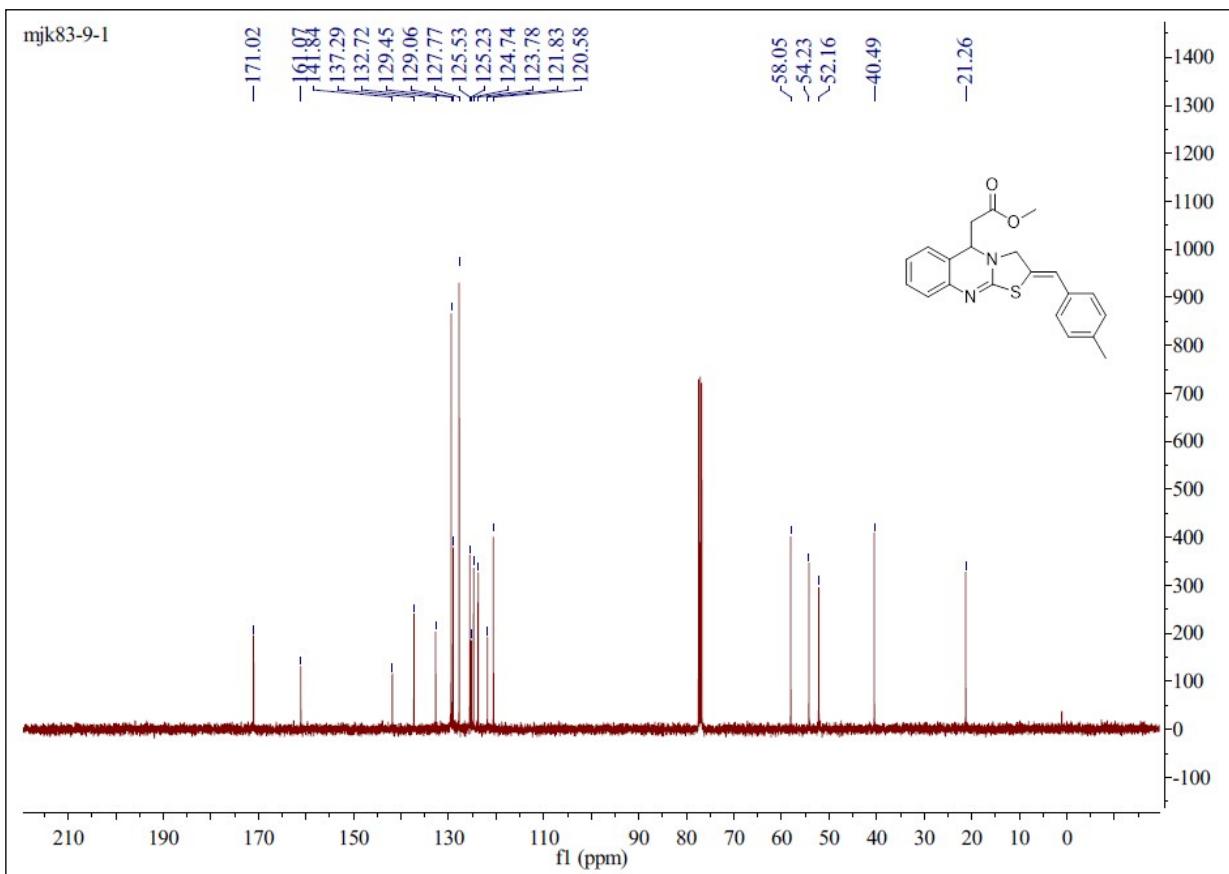
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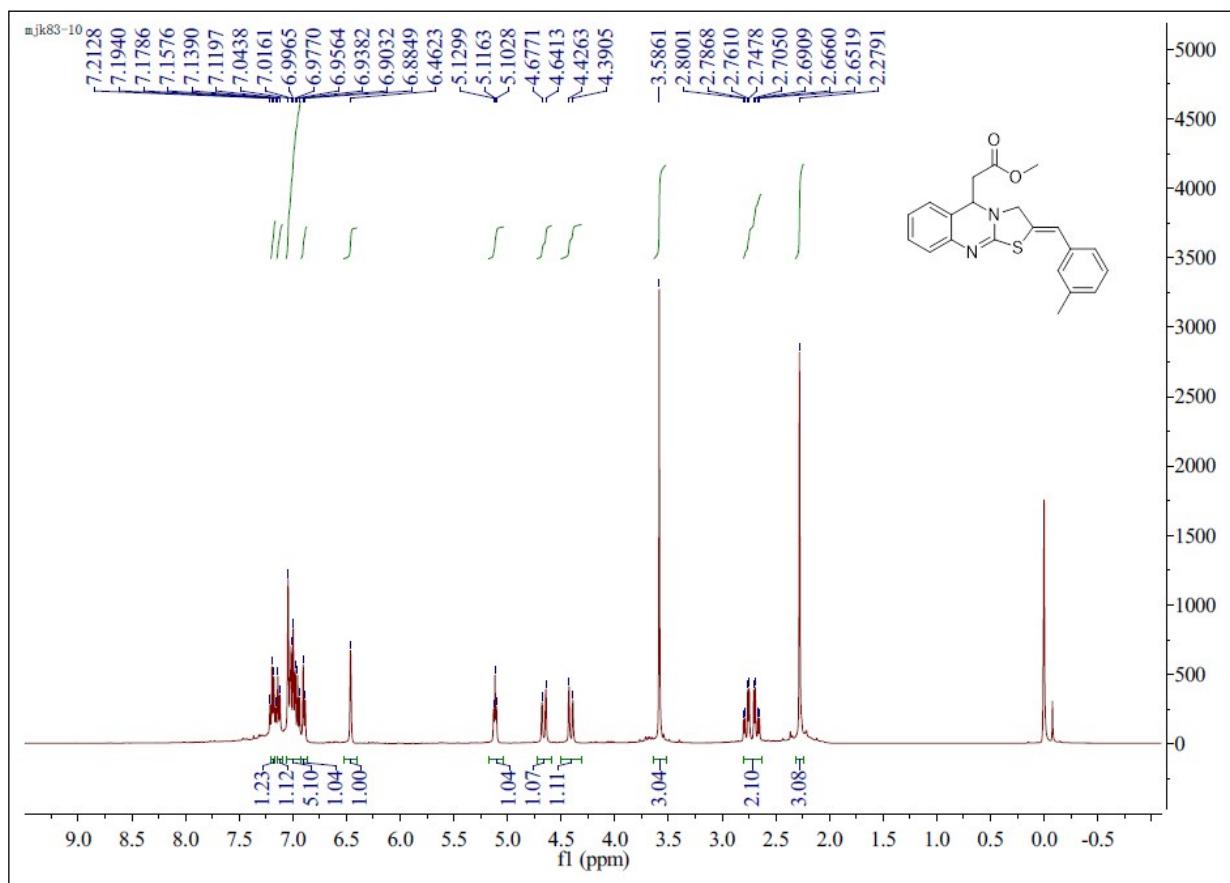
¹H NMR of 3ah



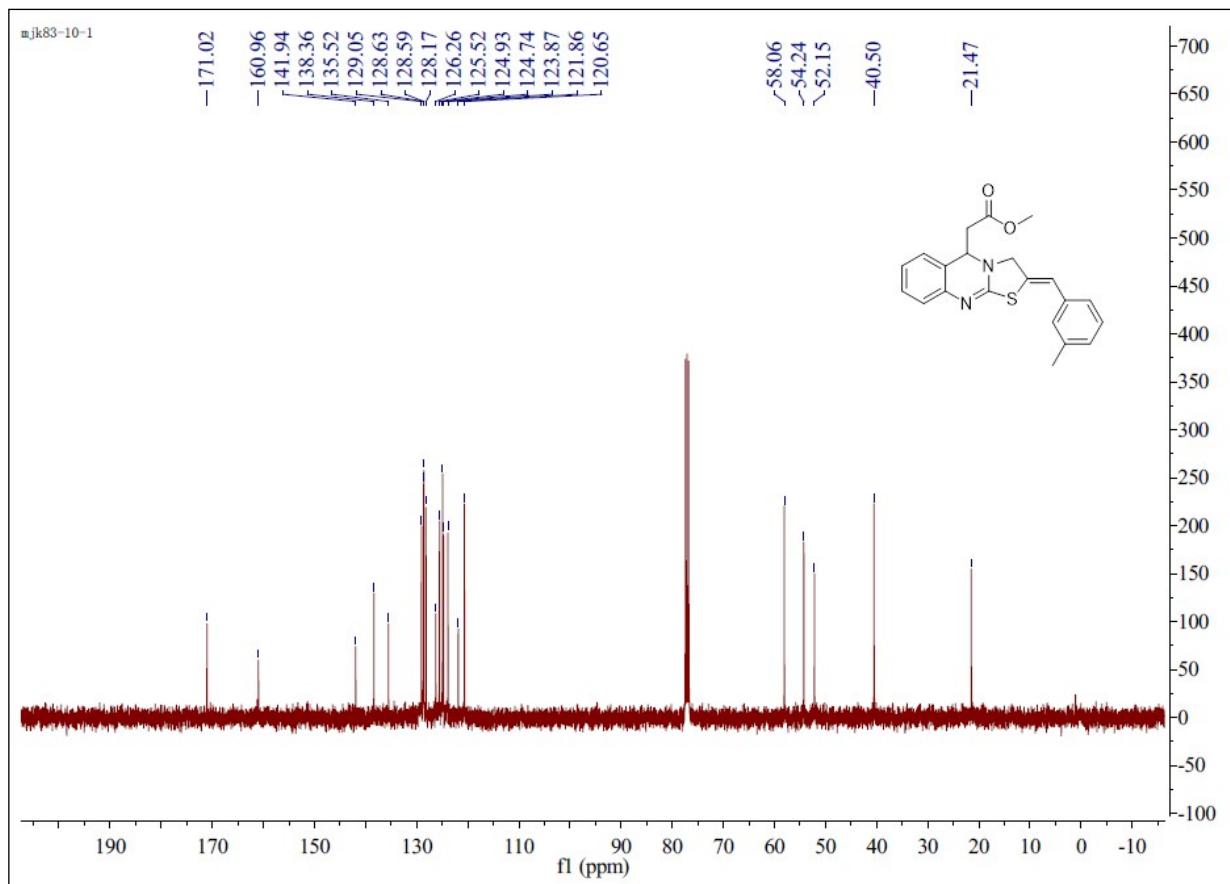
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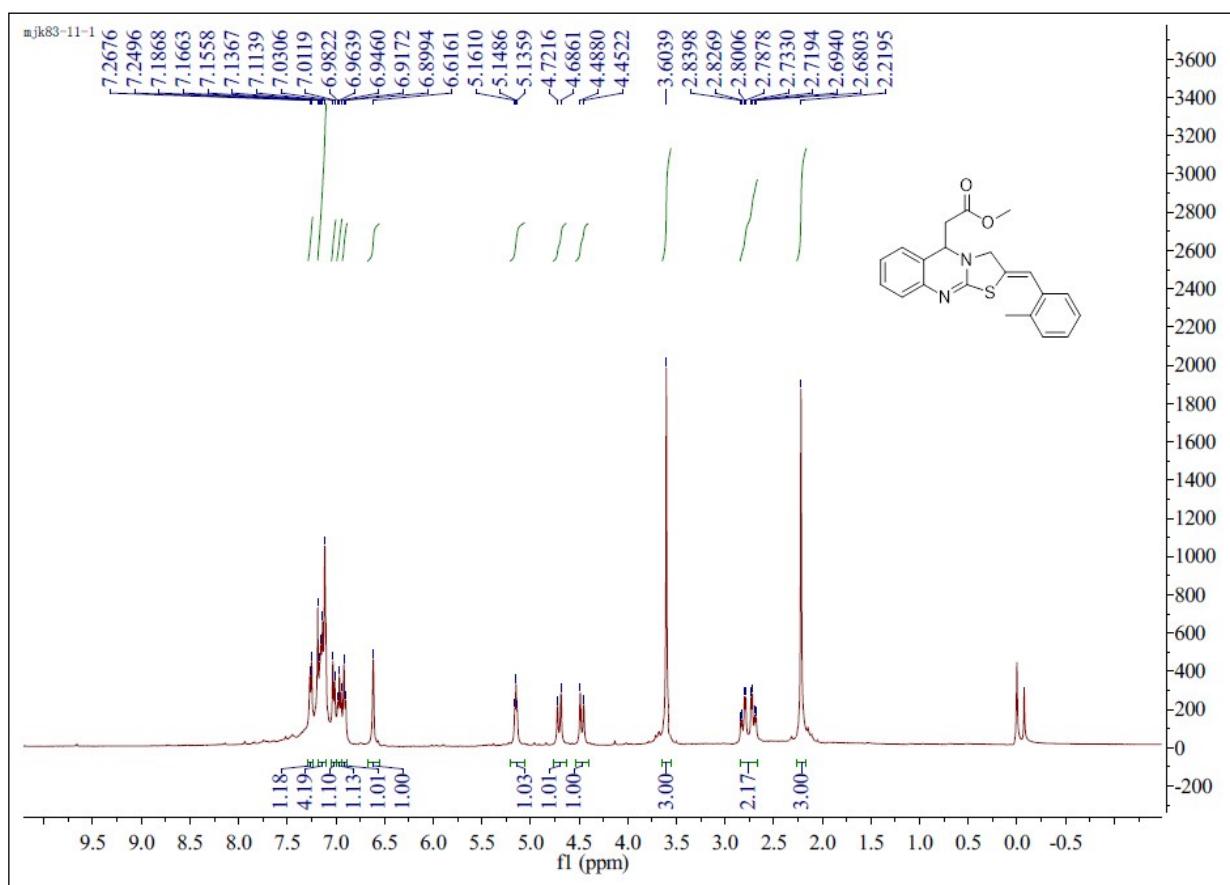
¹H NMR of 3ai



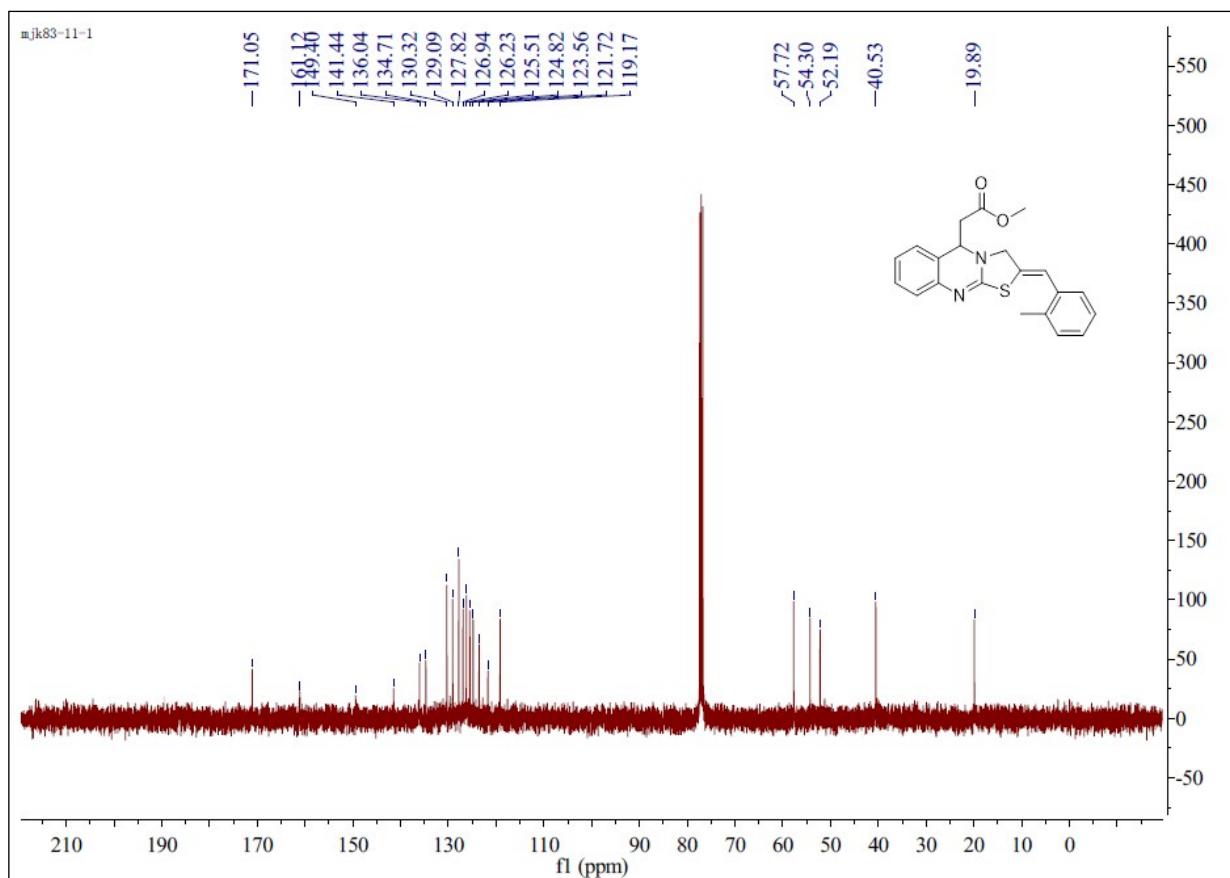
¹³C NMR of 3ai



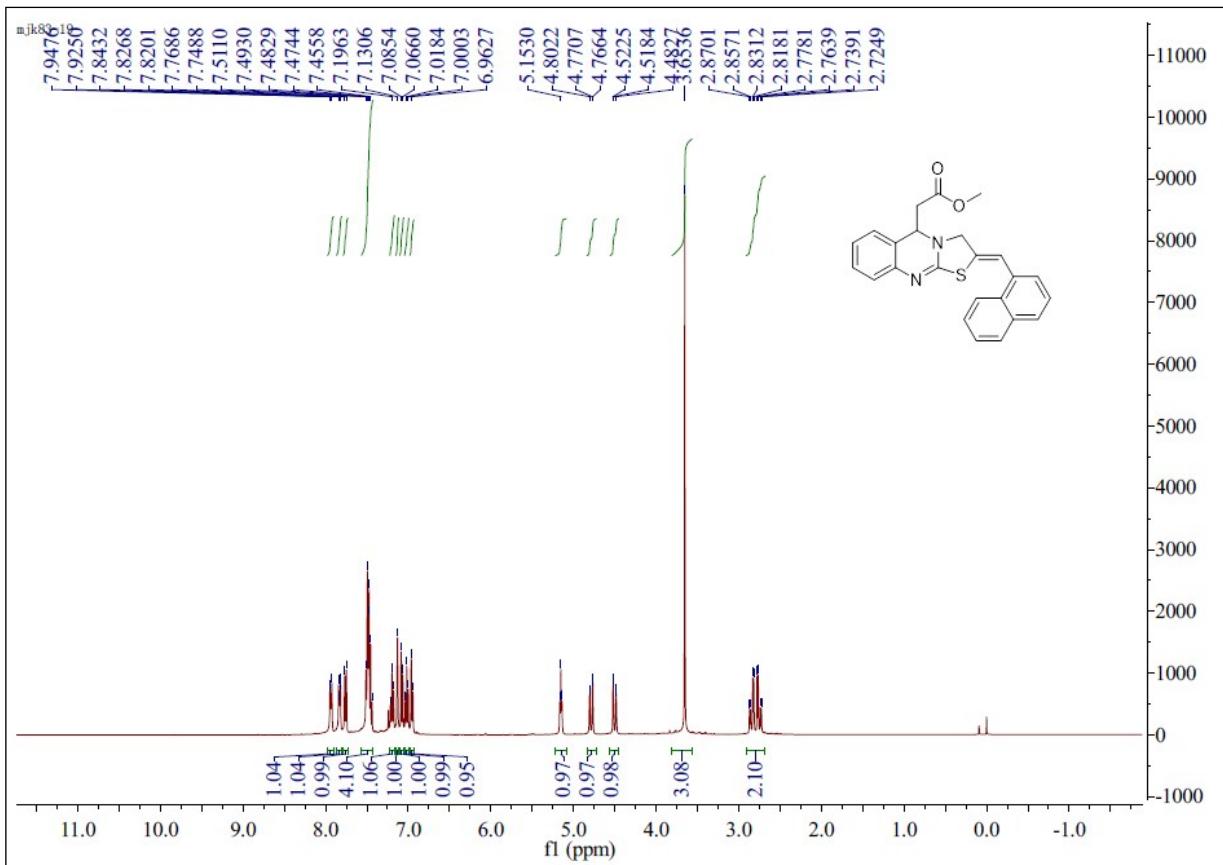
¹H NMR of 3aj



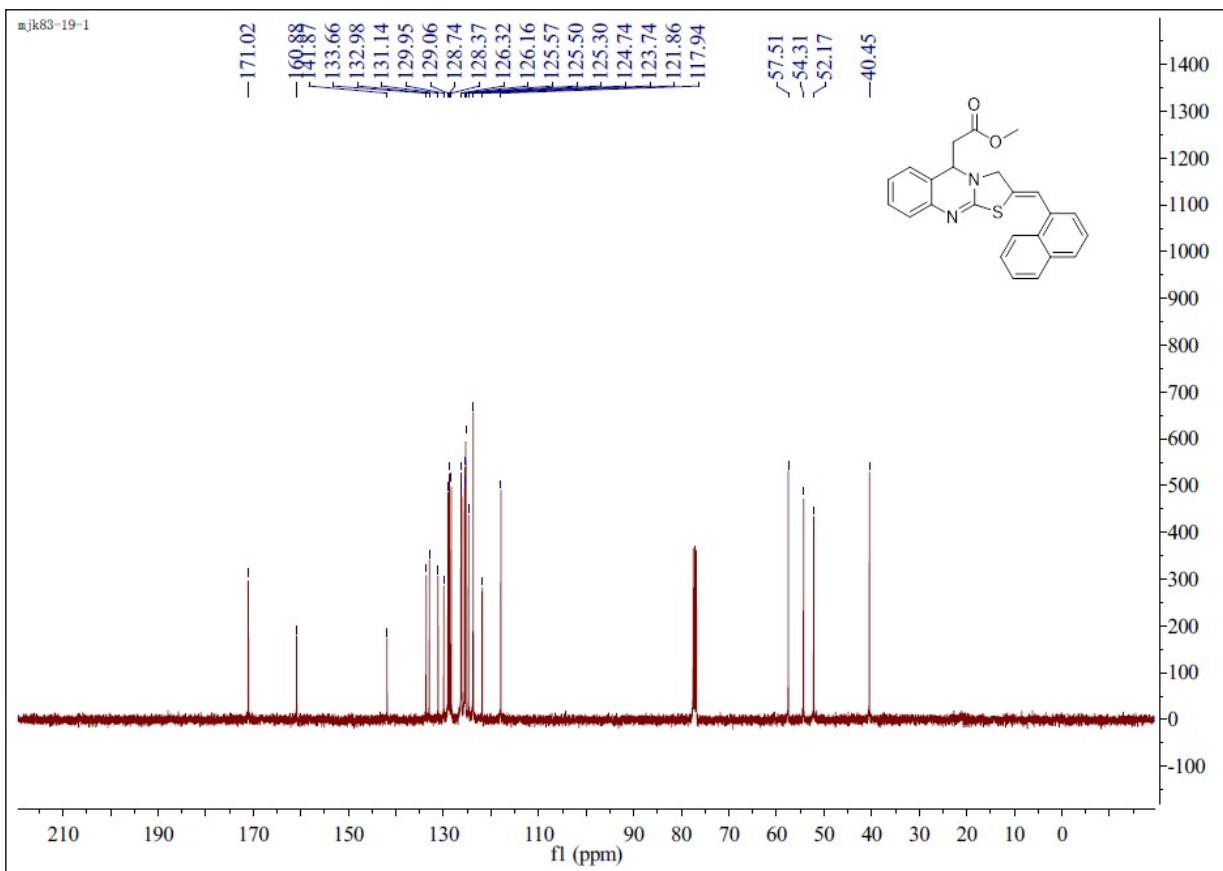
¹H NMR of **3aj**



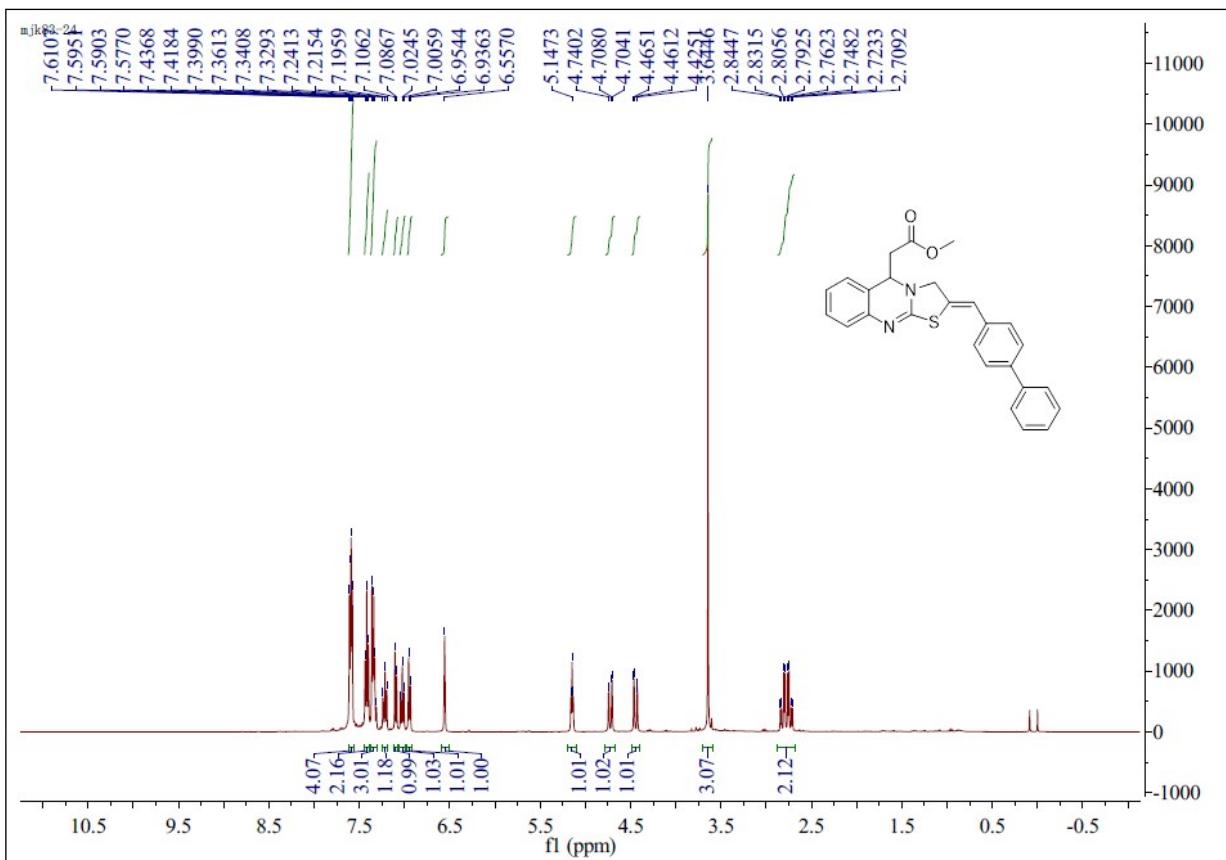
¹H NMR of **3ak**



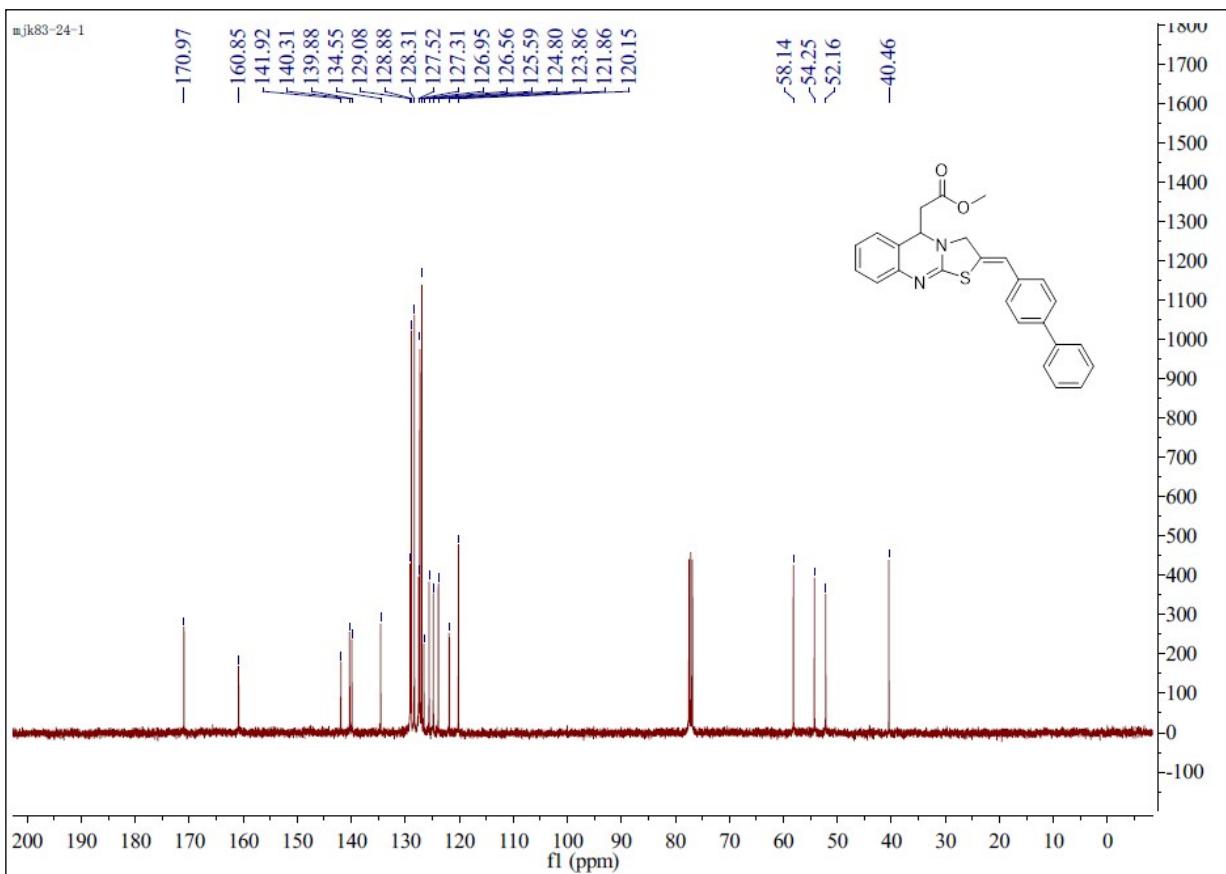
¹³C NMR of 3ak



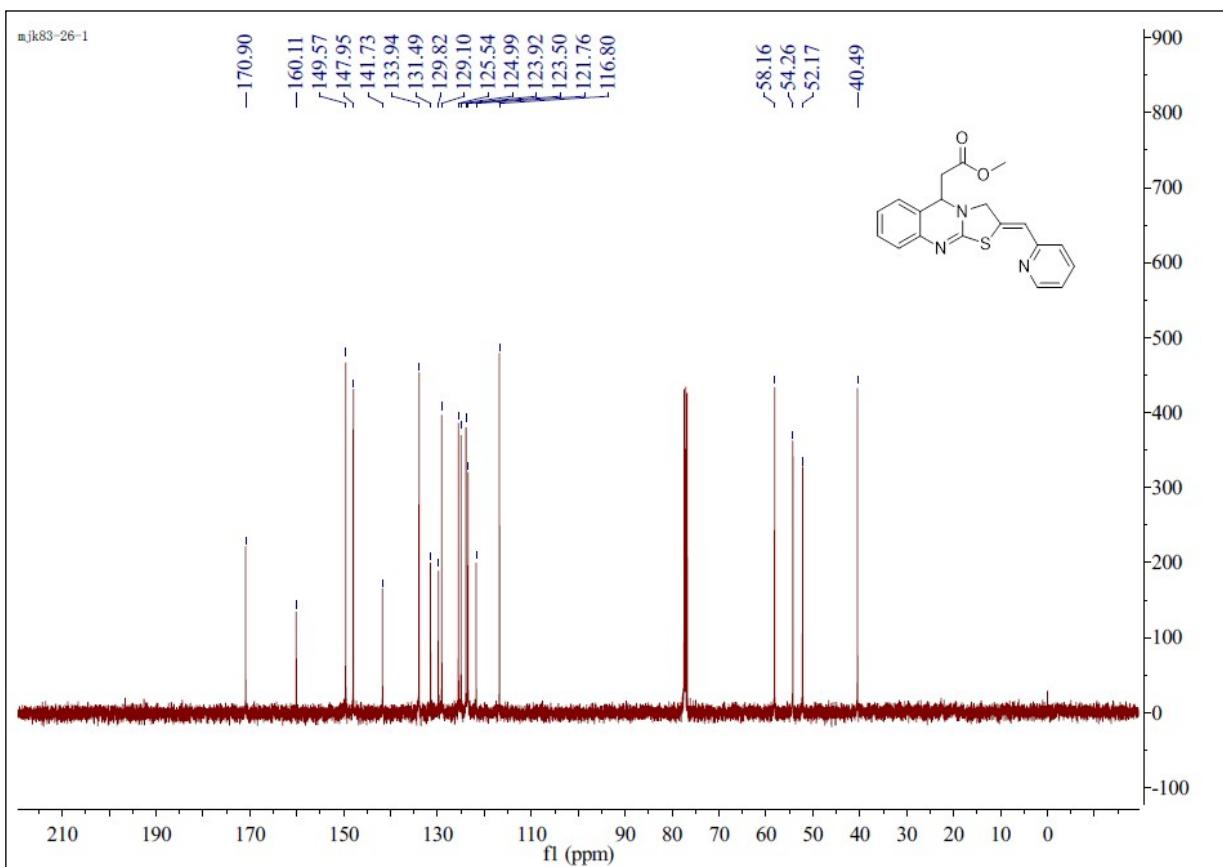
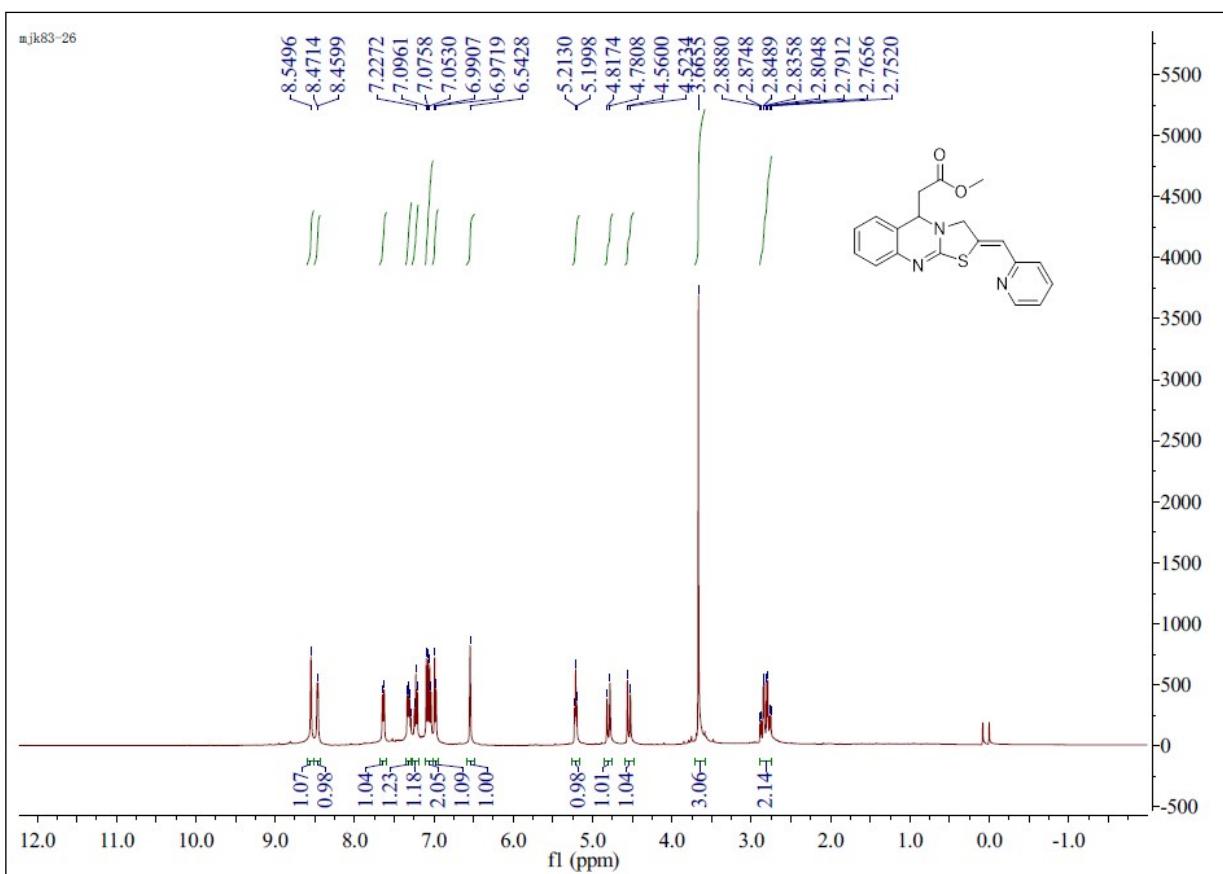
¹H NMR of 3al



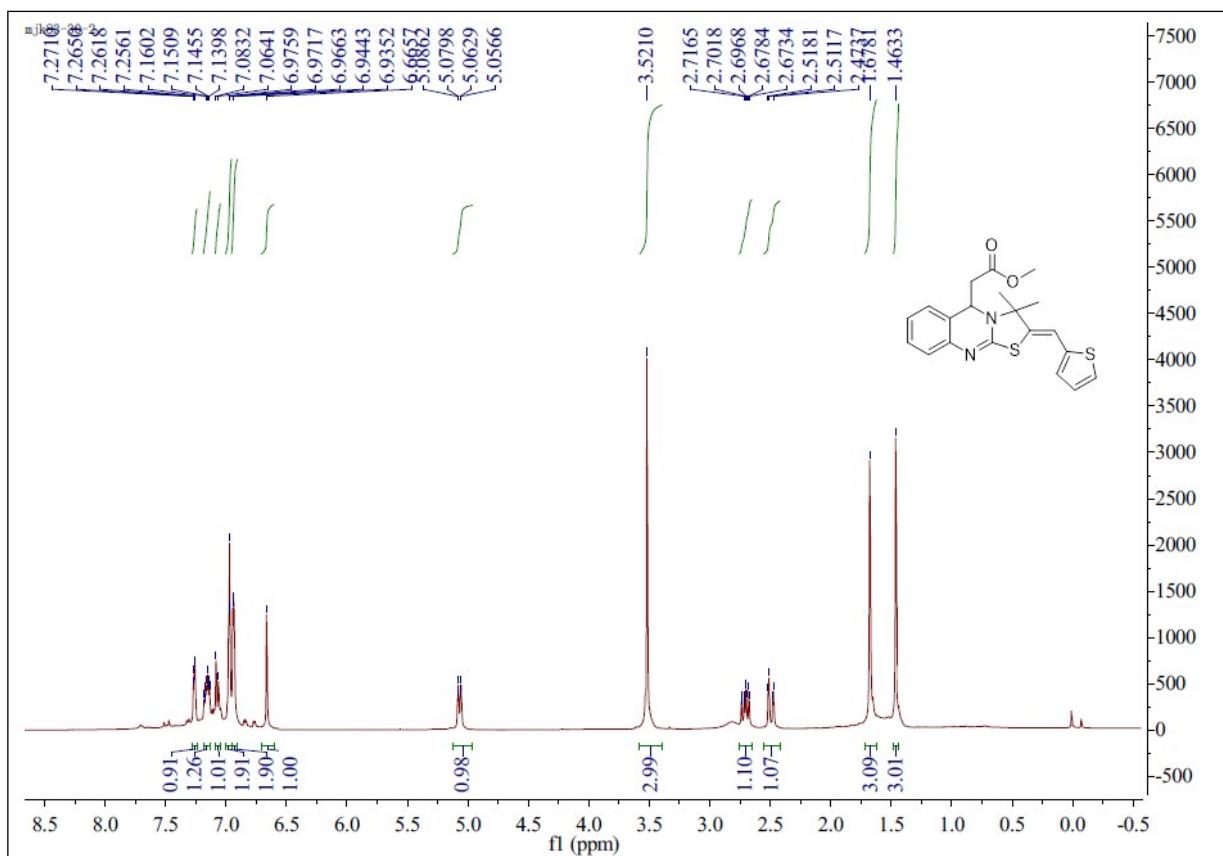
¹³C NMR of **3al**



¹H NMR of 3am



¹H NMR of 3an



¹³C NMR of 3an

