

Supporting Information

Synthesis of novel 1,2,4-triazole derivatives containing the quinazolinylpiperidinyl moiety and *N*-(substituted phenyl)acetamide group as efficient bactericides against the phytopathogenic bacterium *Xanthomonas oryzae* pv. *oryzae*

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***N*-(4-acetylphenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7a)** 59.1 mg, yield: 81%, as a brown solid; mp 119–120 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.65 (s, 1H), 8.56 (s, 1H), 7.91 (d, *J* = 10.0 Hz, 3H), 7.78–7.74 (m, 2H), 7.66 (d, *J* = 5.0 Hz, 2H), 7.60 (d, *J* = 5.0 Hz, 3H), 7.51–7.47 (m, 3H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.14 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.92–2.86 (m, 1H), 2.49 (s, 3H), 1.94–1.83 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 197.1, 166.8, 164.2, 158.6, 154.1, 151.8, 150.4, 143.6, 133.4, 133.2, 132.5, 130.8, 130.7, 130.1, 128.5, 128.0, 126.1, 125.8, 118.9, 116.4, 49.2, 37.4, 32.5, 30.3, 27.0; IR (KBr, ν/cm^{-1}): 1676 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₃₁H₃₀N₇O₂S: 564.2176; found: 564.2179.

***N*-(4-fluorophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7b)** 52.8 mg, yield: 75%, as a white solid; mp 111–113 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.39 (s, 1H), 8.56 (s, 1H), 7.91 (d, *J* = 5.0 Hz, 1H), 7.75 (t, *J* = 5.0 Hz, 2H), 7.61 (d, *J* = 5.0 Hz, 3H), 7.56–7.47 (m, 5H), 7.13 (t, *J* = 5.0 Hz, 2H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.09 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.91–2.86 (m, 1H), 1.94–1.83 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 166.1, 164.2, 158.6, 154.1, 151.6, 150.5, 135.6, 133.3, 130.9, 130.7, 128.3, 128.0, 126.2, 125.8, 121.6, 121.5, 116.3, 116.0, 115.8, 49.2, 37.2, 32.5, 30.2; IR (KBr, ν/cm^{-1}): 1669 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₂₉H₂₇FN₇OS: 540.1976; found: 540.1982.

***N*-(4-bromophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7c)** 68.0 mg, yield: 88%, as a white solid; mp 113–115 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.46 (s, 1H), 8.56 (s, 1H), 7.91 (d, *J* = 5.0 Hz, 1H), 7.78–7.74 (m, 2H), 7.61–7.60 (m, 3H), 7.51–7.46 (m, 7H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.09 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.91–2.85 (m, 1H), 1.94–1.83 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 166.3, 164.2, 158.6, 154.1, 151.8, 150.4, 138.7, 133.4, 133.2, 132.2, 130.8, 130.7, 128.5, 128.0, 126.1, 125.8, 121.6, 116.4, 115.6, 49.2, 37.4, 32.5, 30.3; IR (KBr, ν/cm^{-1}): 1683 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd

for C₂₉H₂₇BrN₇O₃S: 600.1175; found: 600.1177.

N-(4-nitrophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7d) 64.9 mg, yield: 88%, as a pale yellow solid; mp 120–123 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.94 (s, 1H), 8.56 (s, 1H), 8.21 (d, *J* = 10.0 Hz, 2H), 7.91 (d, *J* = 5.0 Hz, 1H), 7.79–7.75 (m, 4H), 7.60–7.58 (m, 3H), 7.51–7.50 (m, 3H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.16 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.92–2.86 (m, 1H), 1.93–1.86 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 167.2, 164.2, 158.7, 154.1, 151.7, 150.3, 145.4, 143.0, 135.6, 133.3, 130.9, 130.7, 128.4, 128.0, 126.2, 125.8, 125.6, 119.4, 116.3, 49.2, 37.4, 32.5, 30.2; IR (KBr, ν/cm⁻¹): 1700 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₂₉H₂₇N₈O₃S: 567.1921; found: 567.1926.

N-(2,4-difluorophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7e) 43.1 mg, yield: 60%, as a white solid; mp 205–206 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.17 (s, 1H), 8.56 (s, 1H), 7.91 (d, *J* = 10.0 Hz, 1H), 7.84–7.78 (m, 1H), 7.76–7.74 (m, 2H), 7.62–7.59 (m, 3H), 7.51–7.47 (m, 3H), 7.31 (t, *J* = 10.0 Hz, 1H), 7.04 (t, *J* = 10.0 Hz, 1H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.13 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.92–2.86 (m, 1H), 1.95–1.84 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 166.8, 164.2, 158.6, 154.1, 151.8, 150.4, 133.4, 133.2, 130.8, 130.7, 128.5, 128.0, 126.1, 125.8, 125.7, 125.6, 116.4, 111.9, 111.8, 111.6, 104.9, 104.7, 104.5, 49.2, 36.9, 32.6, 30.3; IR (KBr, ν/cm⁻¹): 1679 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₂₉H₂₆F₂N₇O₃S: 558.1882; found: 558.1884.

N-(4-(trifluoromethyl)-phenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7f) 58.4 mg, yield: 77%, as a white solid; mp 115–116 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.66 (s, 1H), 8.56 (s, 1H), 7.91 (d, *J* = 10.0 Hz, 1H), 7.78–7.73 (m, 4H), 7.66 (d, *J* = 5.0 Hz, 2H), 7.60 (d, *J* = 5.0 Hz, 3H), 7.51–7.47 (m, 3H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.13 (s, 2H), 3.13 (t, *J* = 10.0 Hz, 2H), 2.92–2.86 (m, 1H), 1.95–1.83 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 166.8, 164.2, 158.6, 154.1, 151.8, 150.4, 142.9, 133.4, 133.2, 130.8, 130.7, 128.5, 128.0, 126.8,

126.7, 126.1, 125.8, 124.2, 123.9, 123.8, 123.6, 119.5, 116.4, 49.2, 37.4, 32.5, 30.3; IR (KBr, ν/cm^{-1}): 1609 (C=O); ESI-HRMS m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{30}\text{H}_{27}\text{F}_3\text{N}_7\text{OS}$: 590.1944; found: 590.1945.

***N*-(3-fluorophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7g)** 48.7 mg, yield: 70%, as a white solid; mp 120–122 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): 10.53 (s, 1H), 8.56 (s, 1H), 7.91 (d, $J = 10.0$ Hz, 1H), 7.78–7.74 (m, 2H), 7.61–7.60 (m, 3H), 7.53–7.48 (m, 4H), 7.35–7.30 (m, 1H), 7.24 (d, $J = 5.0$ Hz, 1H), 6.86 (t, $J = 10.0$ Hz, 1H), 4.20 (d, $J = 15.0$ Hz, 2H), 4.10 (s, 2H), 3.12 (t, $J = 10.0$ Hz, 2H), 2.91–2.87 (m, 1H), 1.94–1.83 (m, 4H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): 166.5, 164.2, 163.6, 161.7, 158.6, 154.2, 151.8, 150.4, 141.1, 133.4, 133.2, 130.8, 130.7, 128.5, 128.0, 126.1, 125.8, 116.4, 115.4, 110.6, 106.5, 49.2, 37.3, 32.5, 30.3; IR (KBr, ν/cm^{-1}): 1683 (C=O); ESI-HRMS m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{29}\text{H}_{27}\text{FN}_7\text{OS}$: 540.1976; found: 540.1979.

***N*-(2,6-difluorophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7h)** 66.1 mg, yield: 92%, as a white solid; mp 258–260 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): 10.09 (s, 1H), 8.57 (s, 1H), 7.92 (d, $J = 15.0$ Hz, 1H), 7.77–7.75 (m, 2H), 7.63–7.58 (m, 3H), 7.51–7.48 (m, 3H), 7.35–7.29 (m, 1H), 7.13 (t, $J = 5.0$ Hz, 2H), 4.21 (d, $J = 15.0$ Hz, 2H), 4.17 (s, 2H), 3.13 (t, $J = 10.0$ Hz, 2H), 2.92–2.87 (m, 1H), 1.96–1.85 (m, 4H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): 166.5, 164.3, 159.0, 158.5, 157.1, 154.2, 151.8, 150.2, 133.4, 133.2, 130.8, 130.7, 128.5, 128.0, 126.1, 125.8, 116.4, 112.5, 112.4, 49.2, 36.2, 32.5, 30.3; IR (KBr, ν/cm^{-1}): 1672 (C=O); ESI-HRMS m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{29}\text{H}_{26}\text{F}_2\text{N}_7\text{OS}$: 558.1882; found: 558.1886.

***N*-(2-nitrophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7i)** 43.2 mg, yield: 59%, as a brown solid; mp 99–100 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): 10.68 (s, 1H), 8.56 (s, 1H), 7.97 (d, $J = 5.0$ Hz, 1H), 7.91 (d, $J = 10.0$ Hz, 1H), 7.79–7.75 (m, 3H), 7.70 (t, $J = 10.0$ Hz, 1H), 7.63–

7.60 (m, 3H), 7.51–7.47 (m, 3H), 7.35 (t, $J = 10.0$ Hz, 1H), 4.20 (d, $J = 15.0$ Hz, 2H), 4.12 (s, 2H), 3.13 (t, $J = 10.0$ Hz, 2H), 2.92–2.87 (m, 1H), 1.95–1.83 (m, 4H); ^{13}C NMR (125 MHz, DMSO- d_6): 166.8, 164.2, 158.7, 154.1, 151.8, 150.0, 142.0, 134.9, 133.4, 133.2, 131.8, 130.8, 130.7, 128.5, 128.0, 126.1, 125.9, 125.8, 125.6, 125.3, 116.4, 49.2, 36.8, 32.5, 30.3; IR (KBr, ν/cm^{-1}): 1696 (C=O); ESI-HRMS m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{29}\text{H}_{27}\text{N}_8\text{O}_3\text{S}$: 567.1921; found: 567.1924.

***N*-(2,6-dimethylphenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7j)** 41.2 mg, yield: 58%, as a white solid; mp 238–240 °C; ^1H NMR (500 MHz, DMSO- d_6): 9.59 (s, 1H), 8.57 (s, 1H), 7.92 (d, $J = 10.0$ Hz, 1H), 7.79–7.75 (m, 2H), 7.64–7.60 (m, 3H), 7.52–7.48 (m, 3H), 7.05–6.99 (m, 3H), 4.22 (d, $J = 15.0$ Hz, 2H), 4.10 (s, 2H), 3.13 (t, $J = 10.0$ Hz, 2H), 2.93–2.87 (m, 1H), 2.06 (s, 6H), 1.94–1.84 (m, 4H); ^{13}C NMR (125 MHz, DMSO- d_6): 165.9, 164.3, 158.5, 154.2, 151.8, 150.4, 135.7, 135.2, 133.5, 133.2, 130.8, 130.7, 128.5, 128.2, 128.1, 127.1, 126.1, 125.8, 116.4, 49.3, 36.4, 32.5, 30.4, 18.5; IR (KBr, ν/cm^{-1}): 1680 (C=O); ESI-HRMS m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{31}\text{H}_{32}\text{N}_7\text{OS}$: 550.2383; found: 550.2386.

***N*-(2-(trifluoromethyl)phenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7k)** 54.9 mg, yield: 72%, as a pink solid; mp 169–172 °C; ^1H NMR (500 MHz, DMSO- d_6): 9.95 (s, 1H), 8.56 (s, 1H), 7.92 (d, $J = 10.0$ Hz, 1H), 7.77–7.76 (m, 2H), 7.70 (d, $J = 10.0$ Hz, 1H), 7.67–7.60 (m, 4H), 7.52–7.47 (m, 4H), 7.42 (t, $J = 10.0$ Hz, 1H), 4.22 (d, $J = 15.0$ Hz, 2H), 4.12 (s, 2H), 3.13 (t, $J = 10.0$ Hz, 2H), 2.93–2.88 (m, 1H), 1.97–1.85 (m, 4H); ^{13}C NMR (125 MHz, DMSO- d_6): 167.4, 164.3, 158.6, 154.1, 151.8, 150.4, 135.5, 133.6, 133.4, 133.2, 130.8, 130.7, 129.9, 128.5, 128.0, 127.3, 126.9, 126.8, 126.1, 125.8, 122.9, 116.1, 49.2, 36.6, 32.5, 30.3; IR (KBr, ν/cm^{-1}): 1695 (C=O); ESI-HRMS m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{30}\text{H}_{27}\text{F}_3\text{N}_7\text{OS}$: 590.1944; found: 590.1944.

***N*-(3-acetylphenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-**

triazol-3-yl)thio)acetamide (7l) 66.1 mg, yield: 91%, as a white solid; mp 165–166 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.52 (s, 1H), 8.56 (s, 1H), 8.12 (s, 1H), 7.91 (d, *J* = 10.0 Hz, 1H), 7.78–7.74 (m, 3H), 7.65 (d, *J* = 10.0 Hz, 1H), 7.62–7.58 (m, 3H), 7.51–7.43 (m, 4H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.11 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.92–2.86 (m, 1H), 2.52 (s, 3H), 1.94–1.83 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 198.1, 166.5, 164.2, 158.6, 154.2, 151.8, 150.4, 139.7, 137.9, 133.4, 133.2, 130.8, 130.7, 129.8, 128.5, 128.1, 126.1, 125.8, 124.2, 124.1, 118.7, 116.4, 49.2, 37.3, 32.5, 30.3, 27.3; IR (KBr, ν/cm⁻¹): 1669 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₃₁H₃₀N₇O₂S: 564.2176; found: 564.2180.

***N*-(4-methoxyphenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7m)** 64.8 mg, yield: 91%, as a white solid; mp 160–163 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.15 (s, 1H), 8.56 (s, 1H), 7.91 (d, *J* = 10.0 Hz, 1H), 7.76 (d, *J* = 5.0 Hz, 2H), 7.60 (d, *J* = 5.0 Hz, 3H), 7.51–7.47 (m, 3H), 7.43 (d, *J* = 10.0 Hz, 2H), 6.85 (d, *J* = 10.0 Hz, 2H), 4.21 (d, *J* = 15.0 Hz, 2H), 4.05 (s, 2H), 3.68 (s, 3H), 3.13 (t, *J* = 10.0 Hz, 2H), 2.92–2.86 (m, 1H), 1.93–1.84 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 165.5, 164.3, 158.5, 155.9, 154.1, 151.8, 150.5, 133.5, 133.2, 132.5, 130.8, 130.7, 128.5, 128.1, 126.1, 125.8, 121.2, 116.4, 114.5, 55.7, 49.2, 37.4, 32.5, 30.3; IR (KBr, ν/cm⁻¹): 1668 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₃₀H₃₀N₇O₂S: 552.2176; found: 552.2182.

***N*-(3-nitrophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7n)** 55.4 mg, yield: 75%, as a white solid; mp 209–211 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.81 (s, 1H), 8.57 (t, *J* = 2.1 Hz, 1H), 8.55 (s, 1H), 7.90 (d, *J* = 10.0 Hz, 2H), 7.84 (d, *J* = 10.0 Hz, 1H), 7.78–7.73 (m, 2H), 7.61–7.58 (m, 4H), 7.52–7.46 (m, 3H), 4.20 (d, *J* = 15.0 Hz, 2H), 4.13 (s, 2H), 3.12 (t, *J* = 10.0 Hz, 2H), 2.93–2.87 (m, 1H), 1.94–1.84 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 167.0, 164.2, 158.6, 154.1, 151.8, 150.3, 148.5, 140.4, 133.4, 133.2, 130.9, 130.8, 130.7, 128.5, 128.0, 126.1, 125.8, 125.6, 118.6, 116.4, 113.7, 49.2, 37.2, 32.5, 30.3; IR (KBr, ν/cm⁻¹): 1680 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₂₉H₂₇N₈O₃S:

567.1921; found: 567.1924.

***N*-(4-chlorophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7o)** 65.9 mg, yield: 92%, as a white solid; mp 115–117 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 7.71 (s, 1H), 7.15 (d, *J* = 10.0 Hz, 1H), 6.97–6.96 (m, 2H), 6.81–6.78 (m, 4H), 6.73–6.69 (m, 3H), 6.67–6.65 (m, 2H), 6.47 (d, *J* = 10.0 Hz, 2H), 3.59 (d, *J* = 15.0 Hz, 2H), 3.17 (s, 2H), 2.33 (d, *J* = 10.0 Hz, 2H), 2.20–2.14 (m, 1H), 1.27–1.14 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 166.0, 163.8, 158.2, 152.5, 150.5, 150.0, 136.3, 132.1, 132.0, 129.7, 129.2, 128.1, 127.7, 126.7, 126.1, 124.9, 124.5, 120.2, 115.4, 48.3, 35.7, 32.2, 29.1. IR (KBr, ν/cm⁻¹): 1688 (C=O). ESI-HRMS *m/z*: [M + H]⁺ calcd for C₂₉H₂₇ClN₇OS: 556.1680; found: 556.1687.

***N*-(2,4-dichlorophenyl)-2-((4-phenyl-5-(1-(quinazolin-4-yl)piperidin-4-yl)-4H-1,2,4-triazol-3-yl)thio)acetamide (7p)** 44.0 mg, yield: 58%, as a brown solid; mp 90–92 °C; ¹H NMR (500 MHz, DMSO-*d*₆): 10.01 (s, 1H), 8.53 (s, 1H), 7.88 (d, *J* = 10.0 Hz, 1H), 7.77–7.73 (m, 3H), 7.61–7.57 (m, 4H), 7.48–7.45 (m, 3H), 7.37–7.35 (m, 1H), 4.18 (d, *J* = 15.0 Hz, 2H), 4.12 (s, 2H), 3.09 (t, *J* = 10.0 Hz, 2H), 2.89–2.84 (m, 1H), 1.92–1.81 (m, 4H); ¹³C NMR (125 MHz, DMSO-*d*₆): 167.0, 164.2, 158.6, 154.2, 151.8, 150.4, 134.4, 133.4, 133.2, 130.9, 130.7, 129.8, 129.5, 128.5, 128.2, 128.0, 127.0, 126.6, 126.1, 125.8, 116.4, 49.2, 36.8, 32.5, 30.3; IR (KBr, ν/cm⁻¹): 1688 (C=O); ESI-HRMS *m/z*: [M + H]⁺ calcd for C₂₉H₂₆Cl₂N₇OS: 590.1291; found: 590.1293.

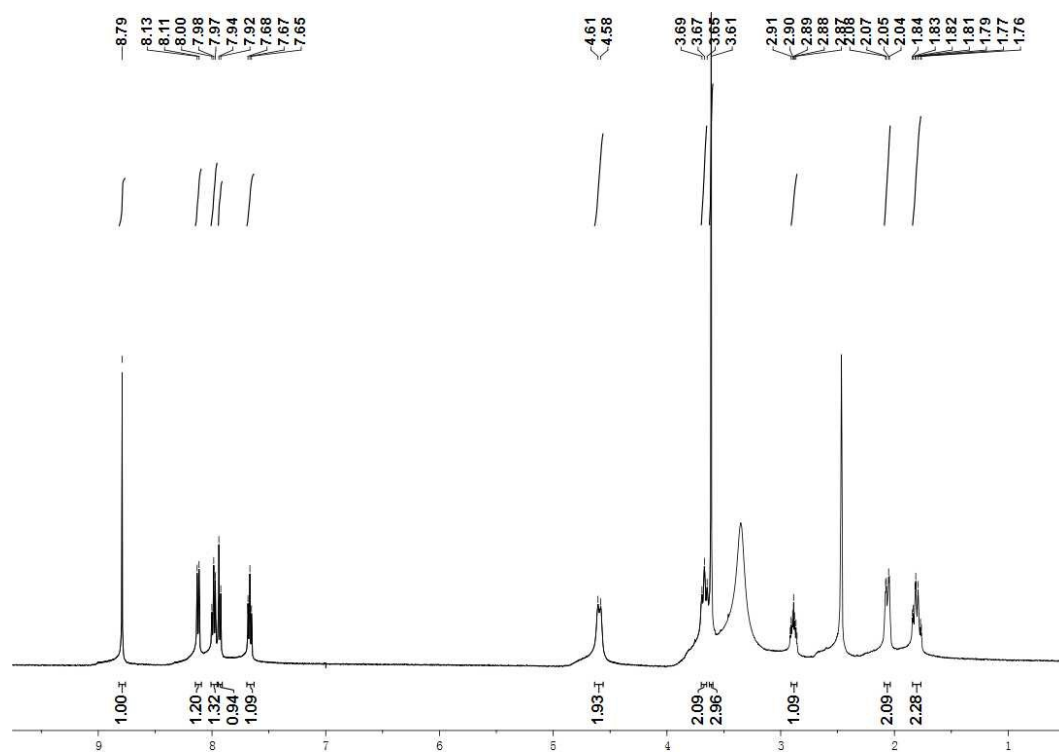


Figure S1. ¹H NMR spectrum of intermediate **2** (DMSO-*d*₆)

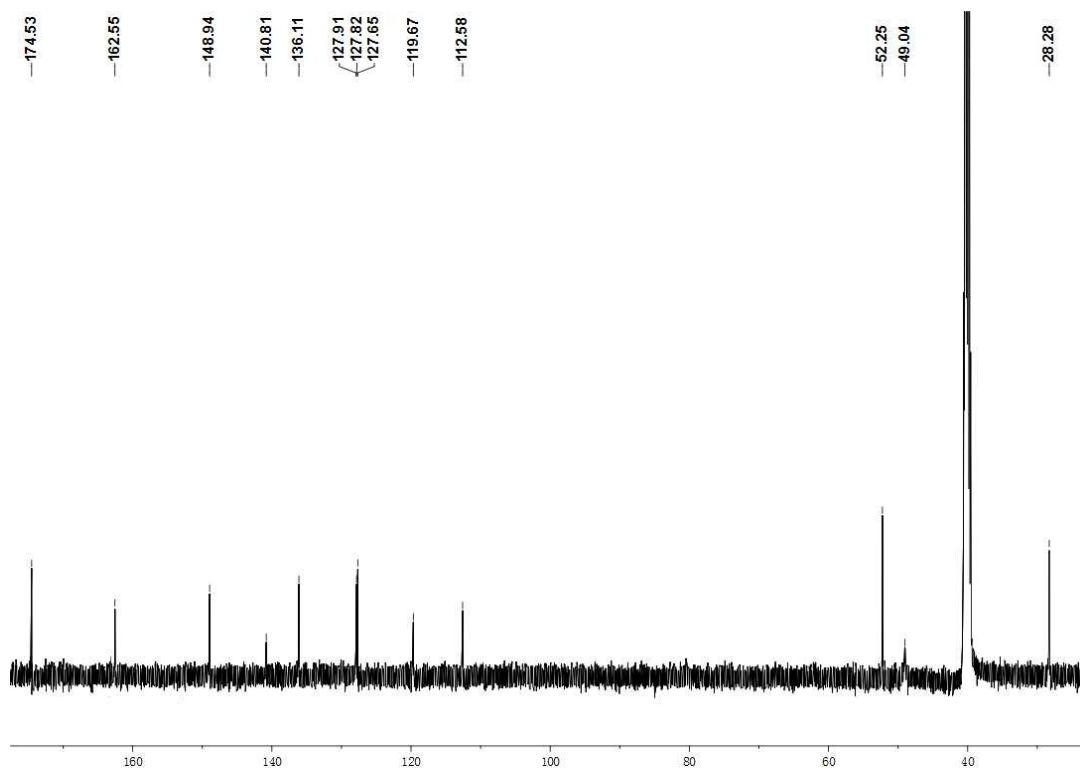


Figure S2. ¹³C NMR spectrum of intermediate **2** (DMSO-*d*₆)

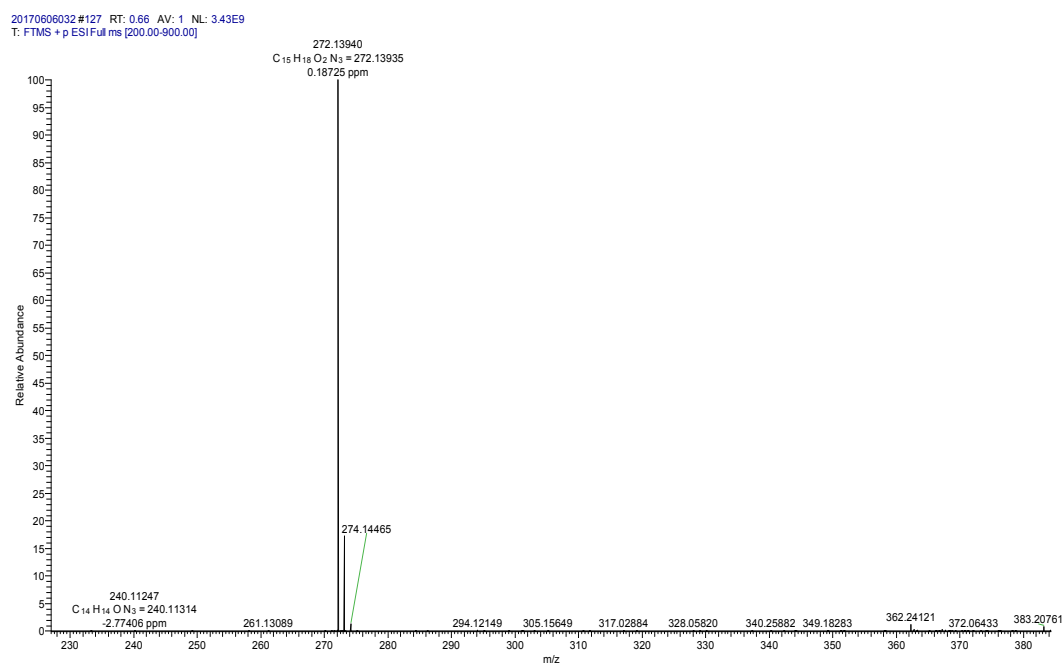


Figure S3. HRMS-ESI spectrum of intermediate **2**

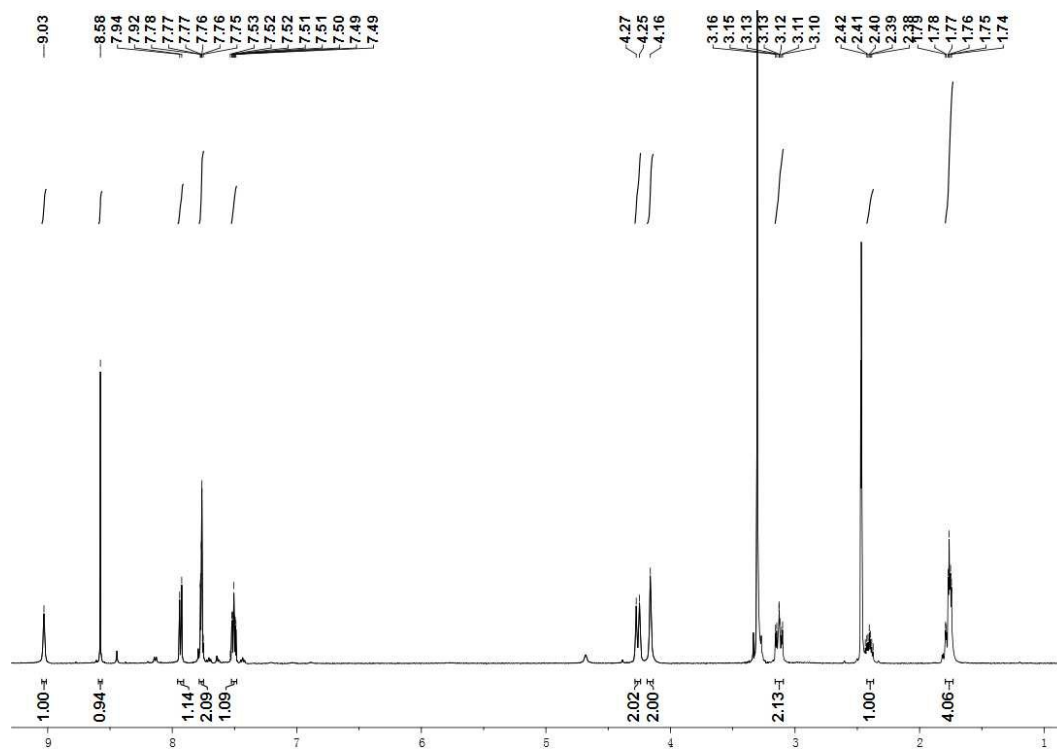


Figure S4. ¹H NMR spectrum of intermediate **3** (DMSO-*d*₆)

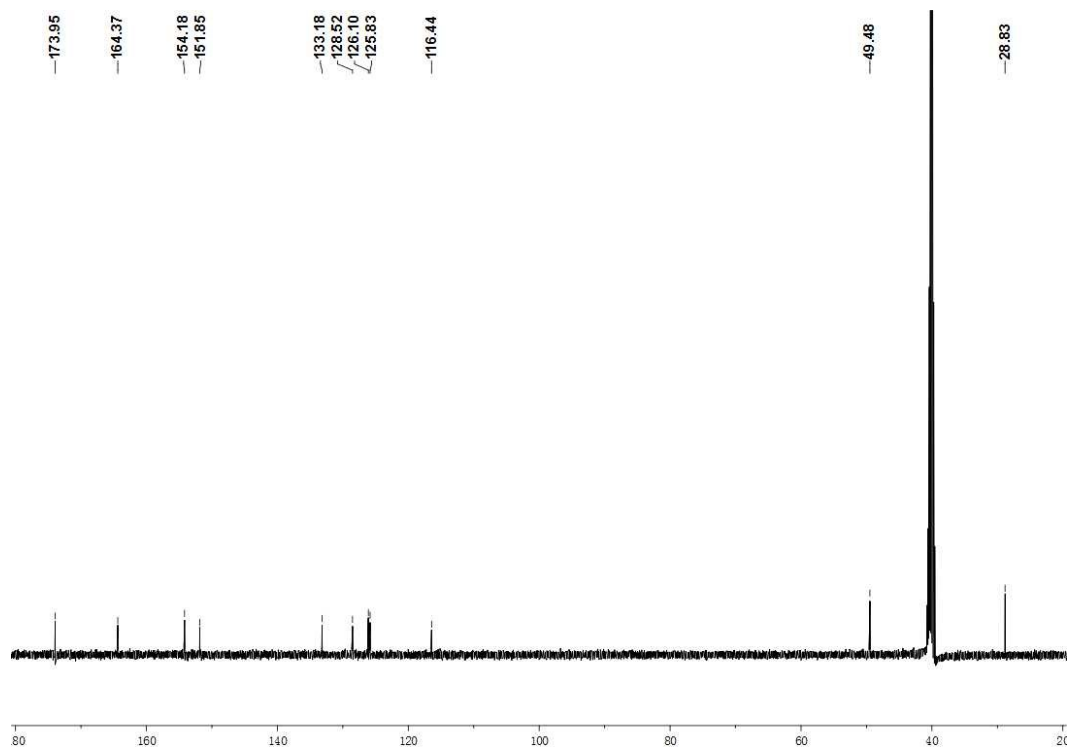


Figure S5. ^{13}C NMR spectrum of intermediate **3** ($\text{DMSO}-d_6$)

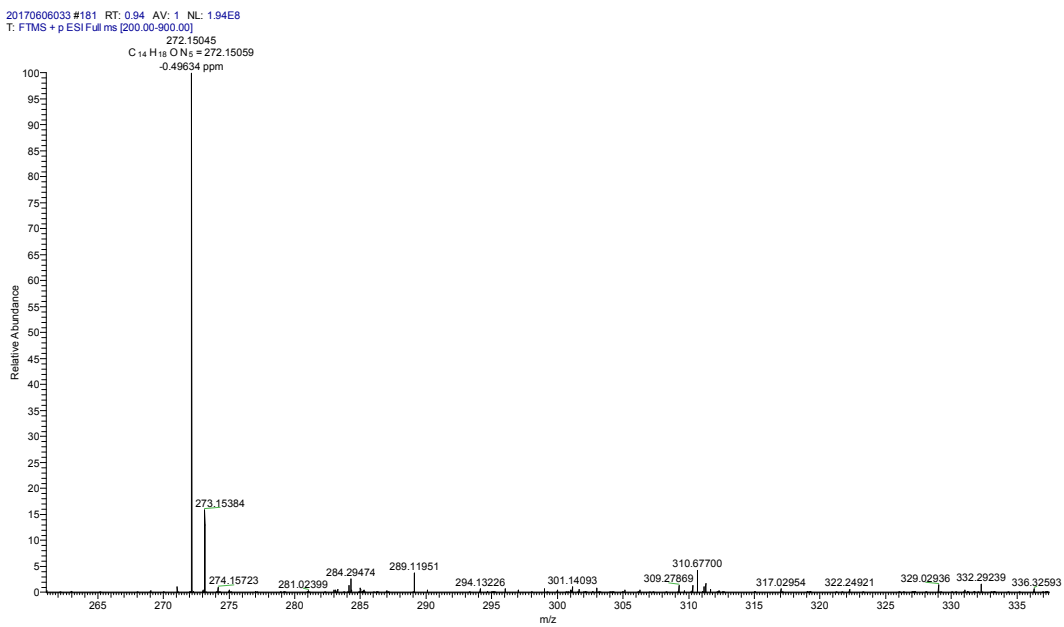


Figure S6. HRMS-ESI spectrum of intermediate **3**

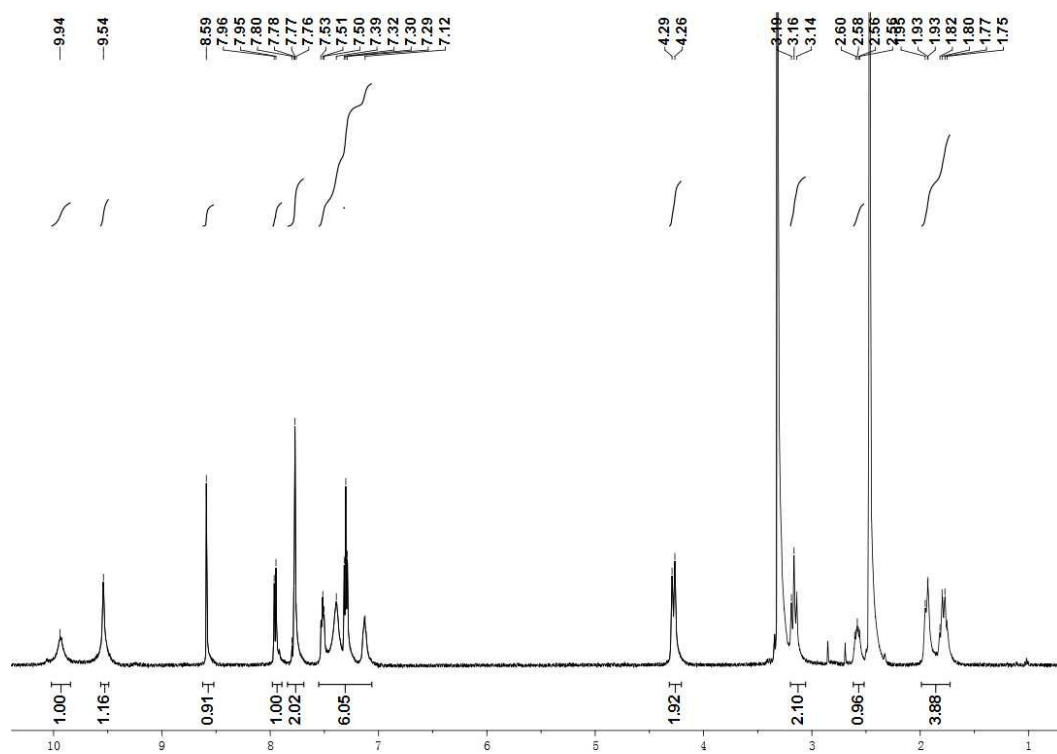


Figure S7. ¹H NMR spectrum of intermediate 4 (DMSO-*d*₆)

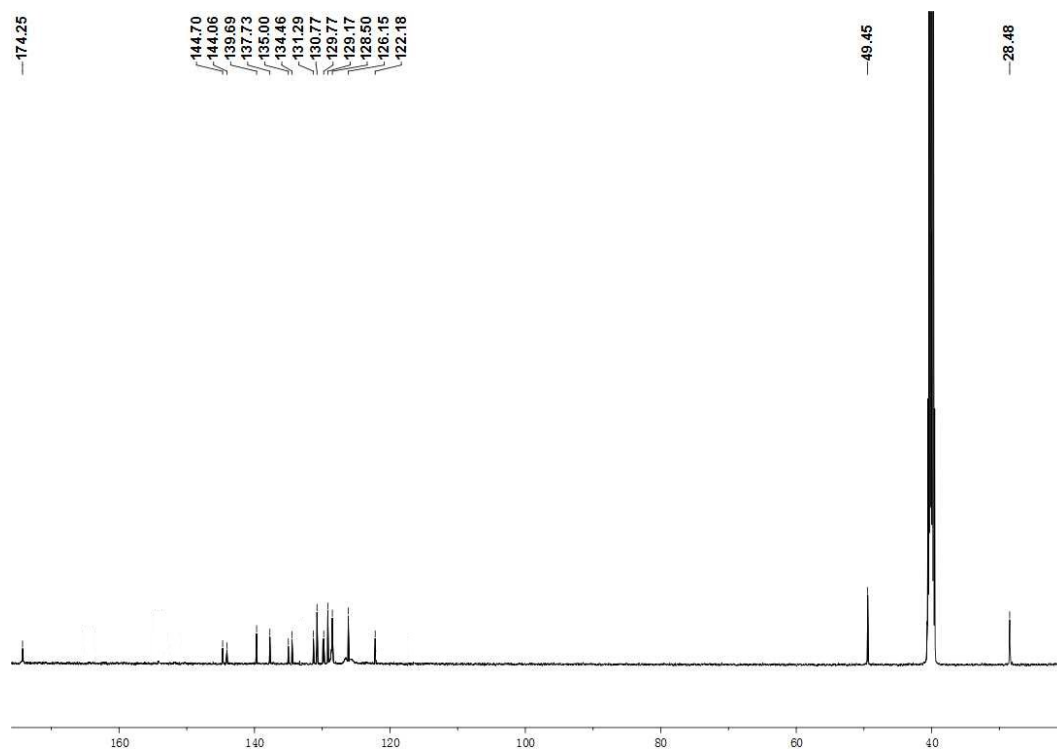


Figure S8. ¹³C NMR spectrum of intermediate 4 (DMSO-*d*₆)

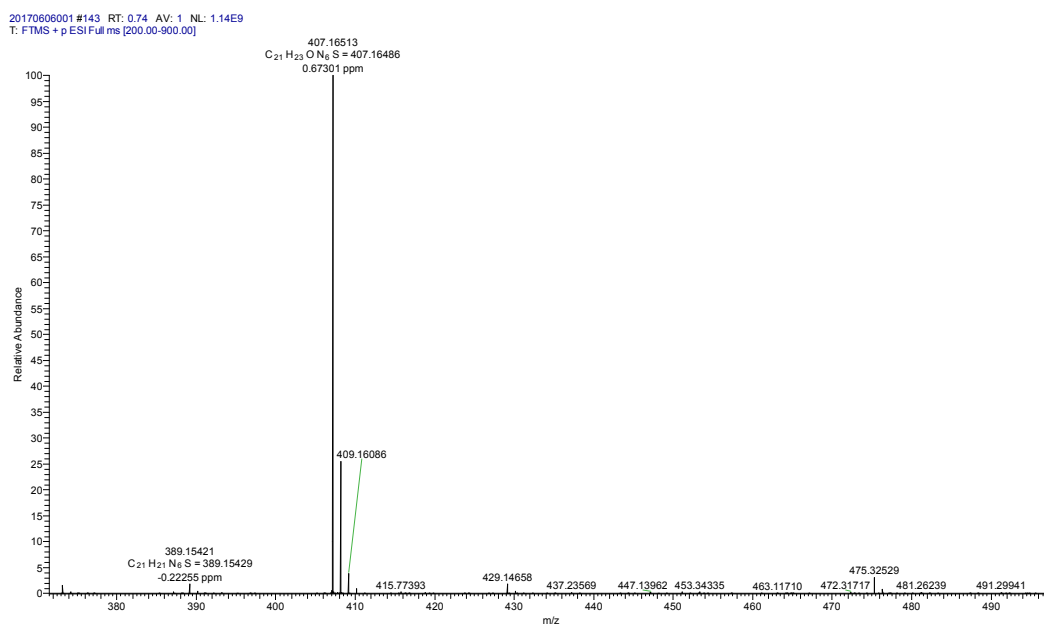


Figure S9. HRMS-ESI spectrum of intermediate **4**

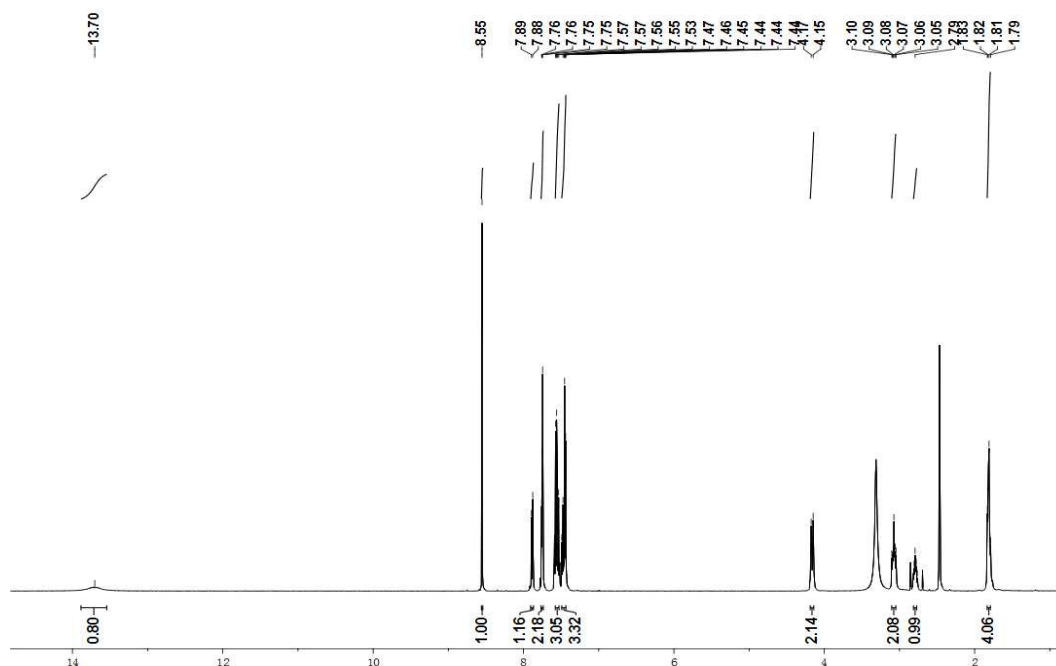


Figure S10. 1H NMR spectrum of intermediate **5** ($DMSO-d_6$)

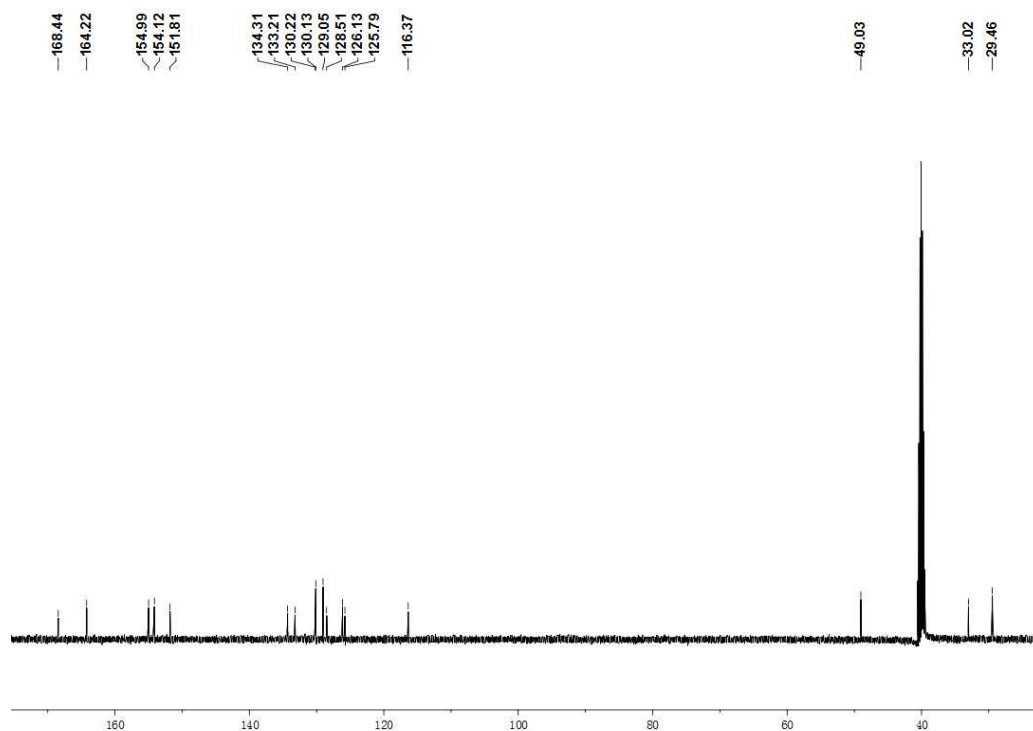


Figure S11. ^{13}C NMR spectrum of intermediate **5** ($\text{DMSO}-d_6$)

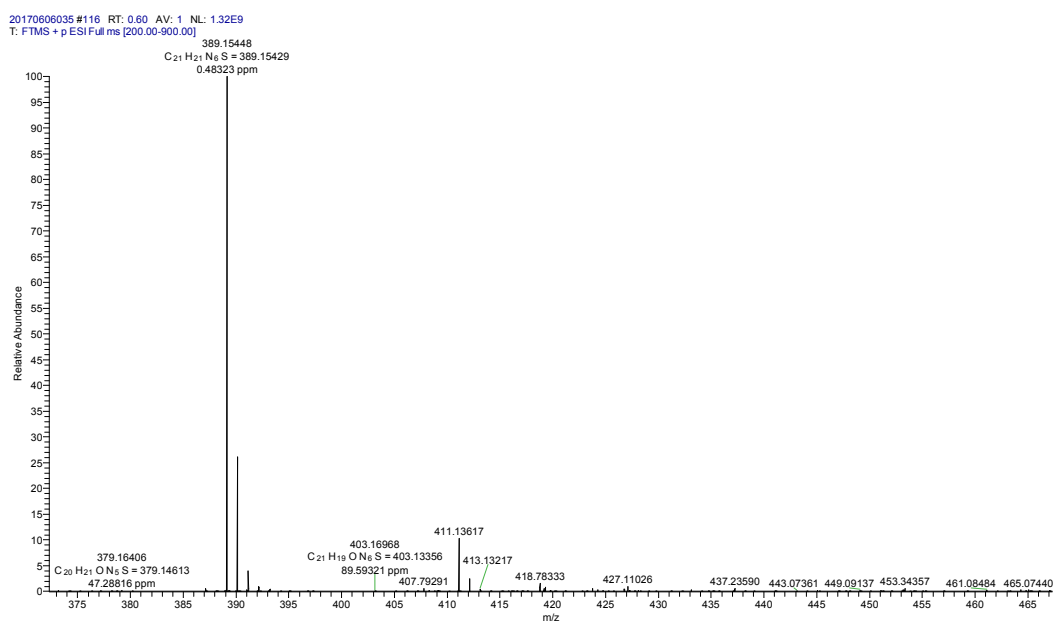


Figure S12. HRMS-ESI spectrum of intermediate **5**

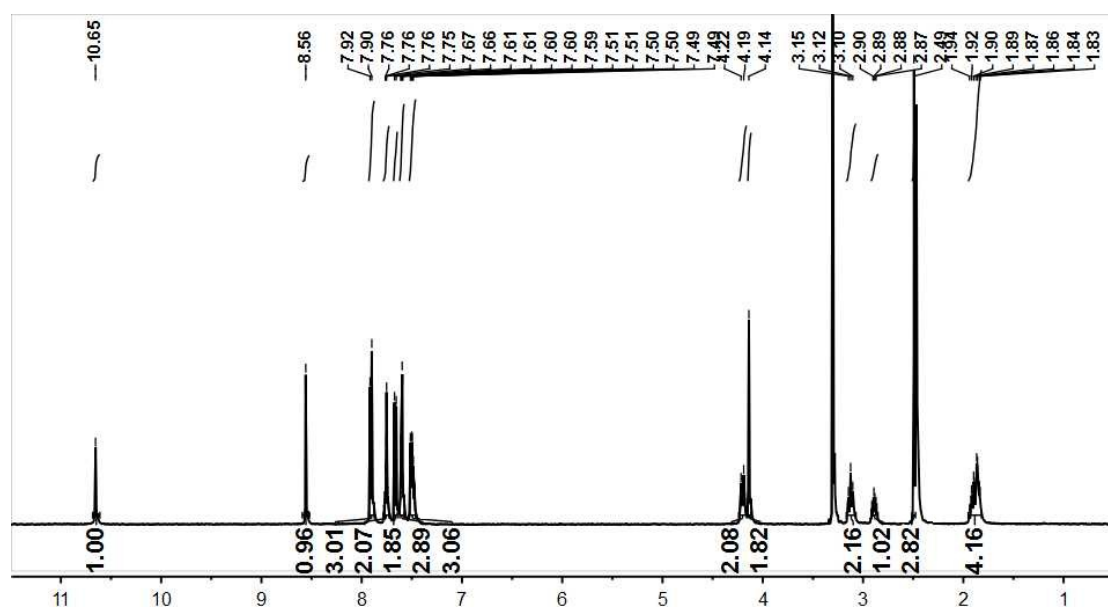


Figure S13. ^1H NMR spectrum of compound **7a** ($\text{DMSO}-d_6$)

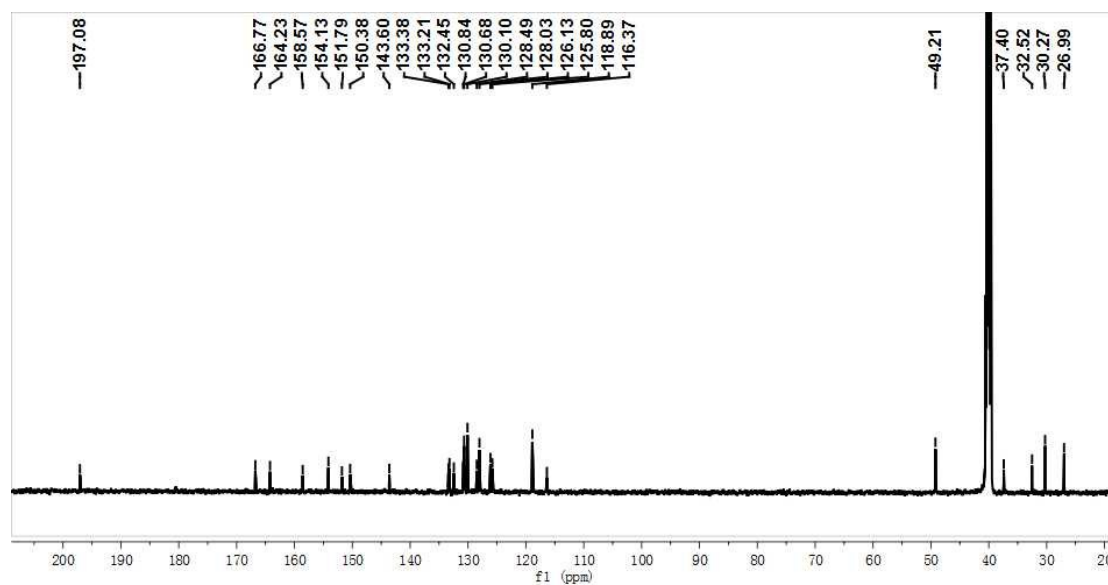


Figure S14. ^{13}C NMR spectrum of compound **7a** ($\text{DMSO}-d_6$)

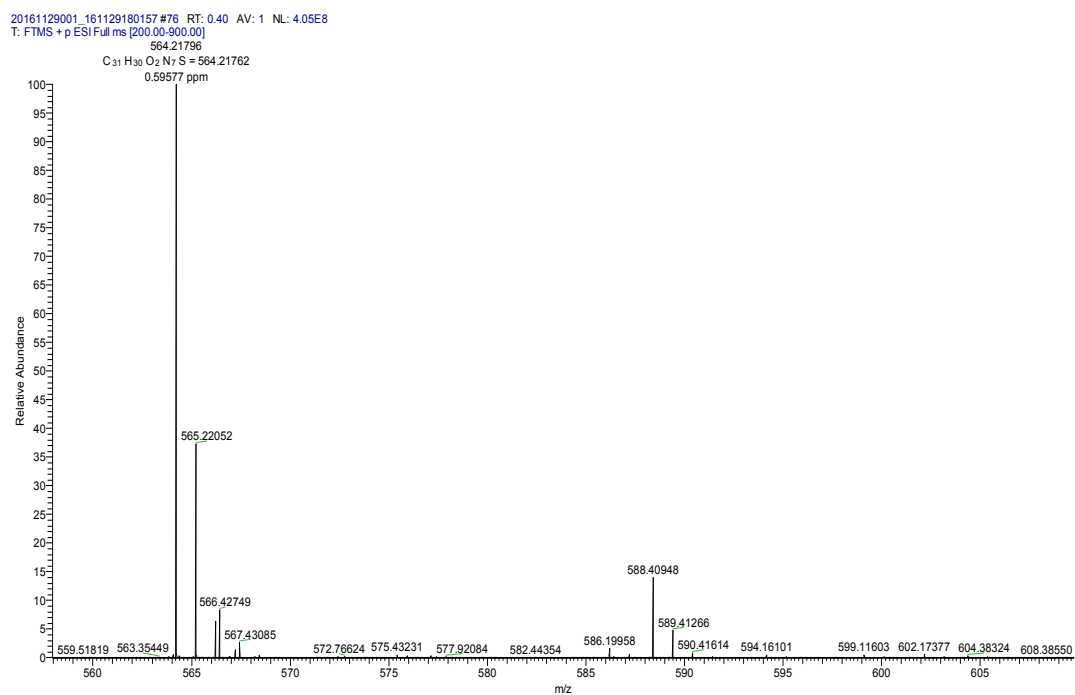


Figure S15. HRMS-ESI spectrum of compound **7a**

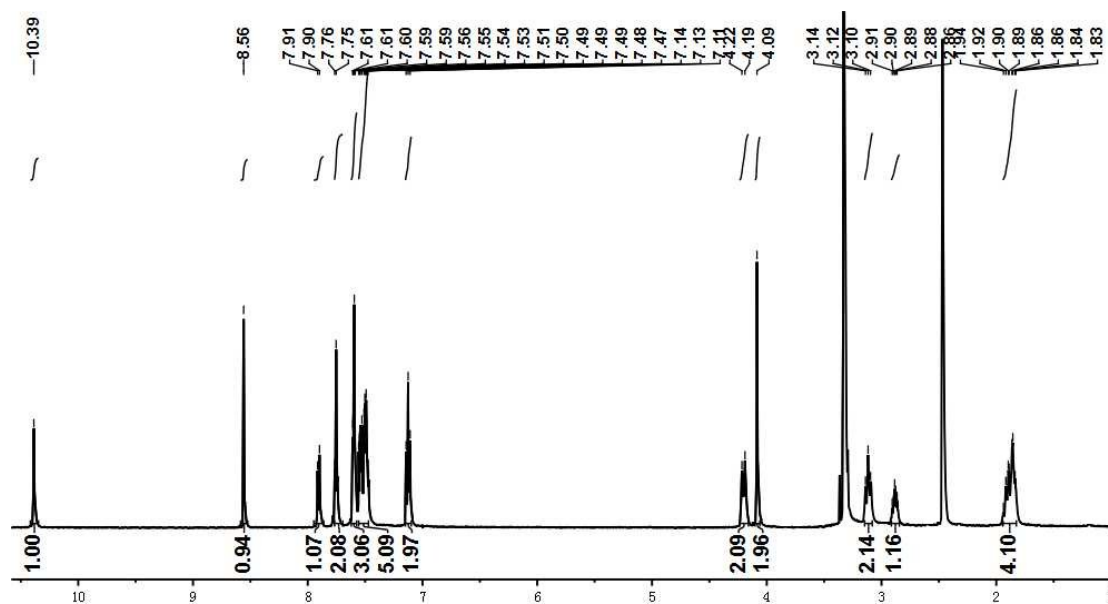


Figure S16. ¹H NMR spectrum of compound **7b** (DMSO-*d*₆)

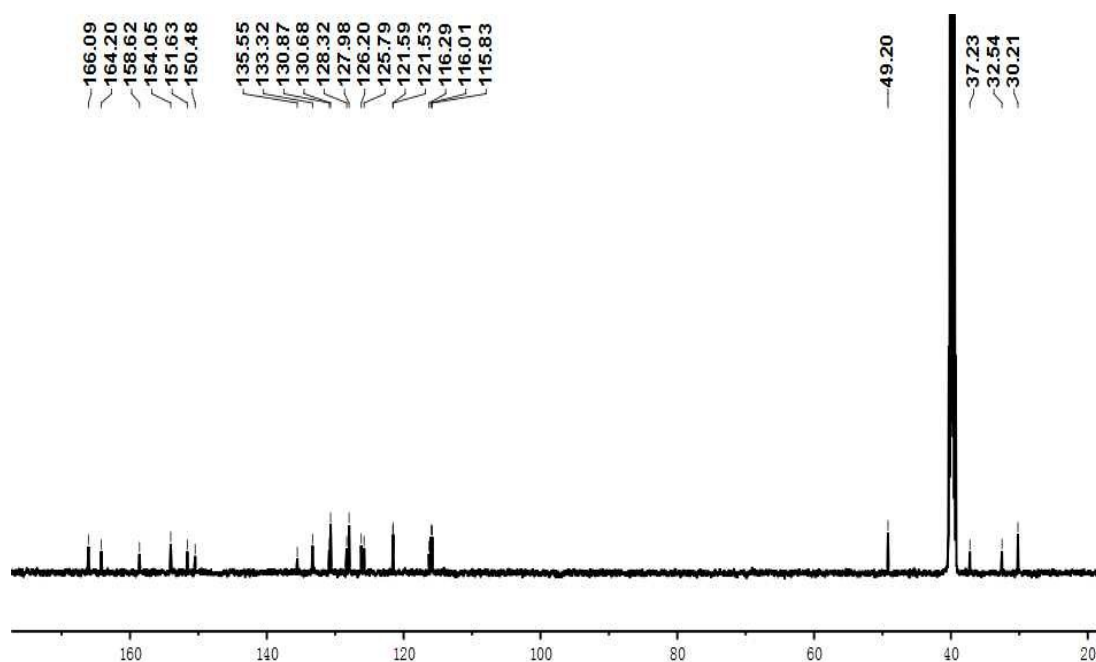


Figure S17. ^{13}C NMR spectrum of compound **7b** ($\text{DMSO}-d_6$)

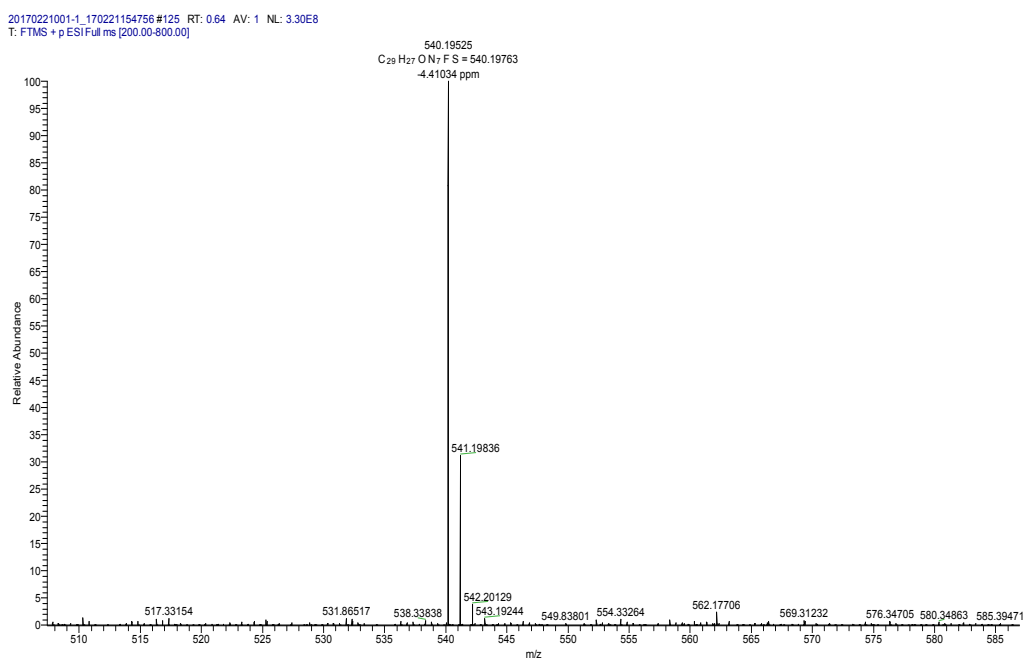


Figure S18. HRMS-ESI spectrum of compound **7b**

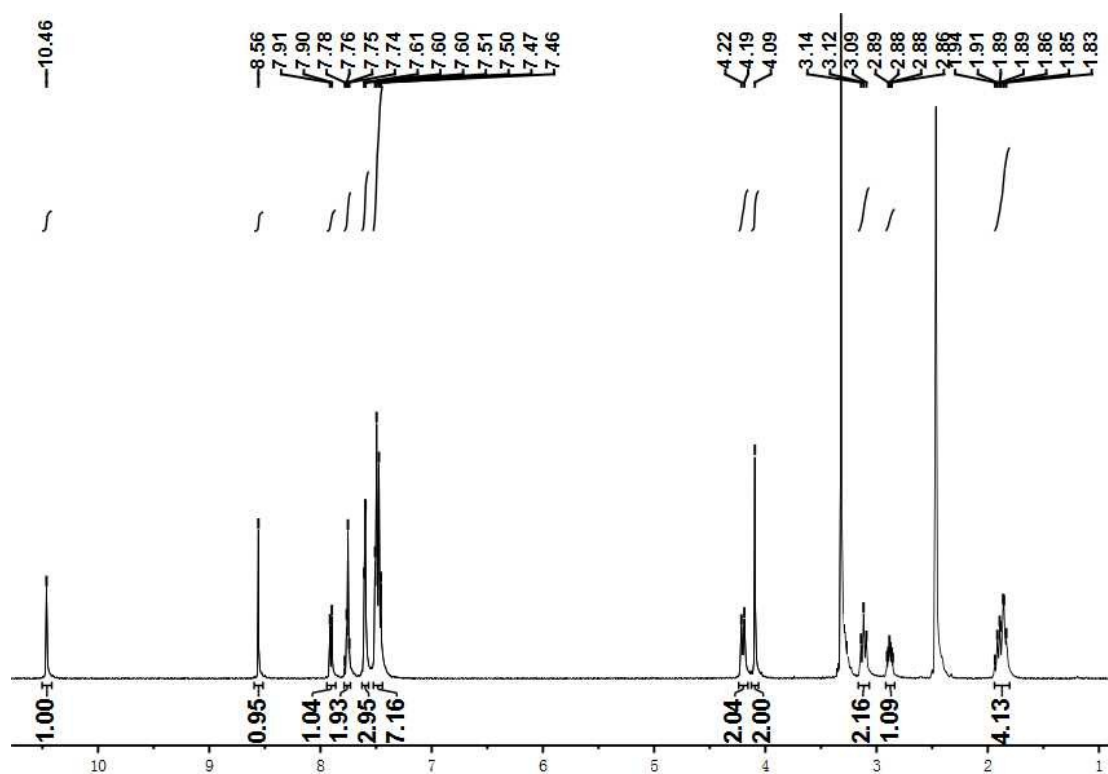


Figure S19. ¹H NMR spectrum of compound 7c (DMSO-*d*₆)

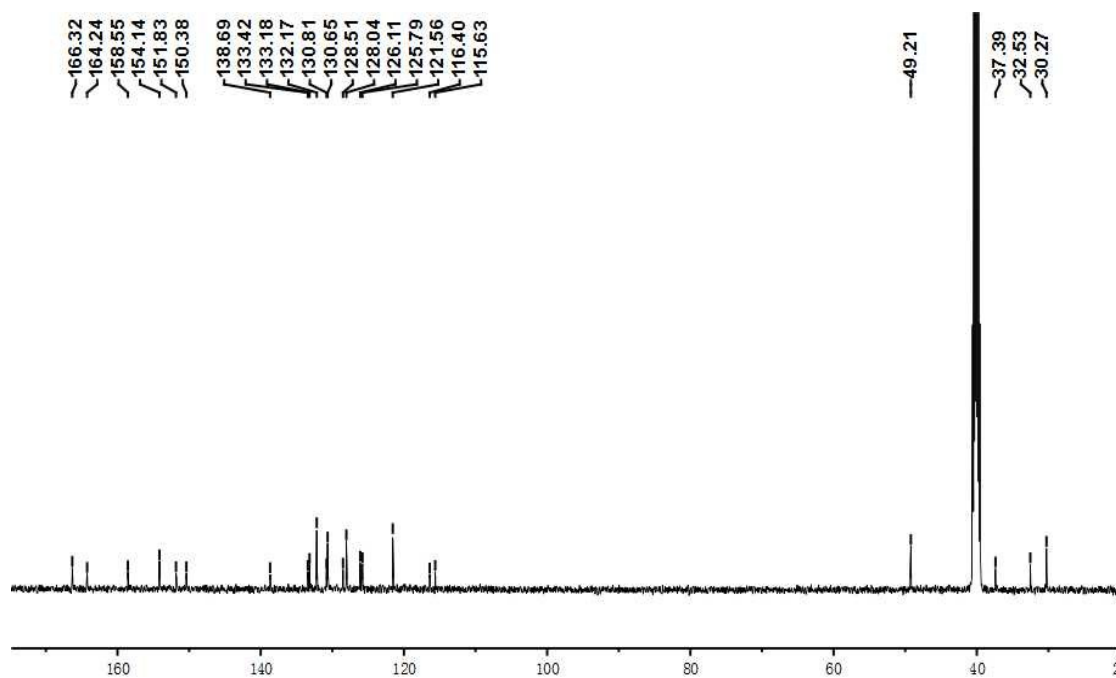


Figure S20. ¹³C NMR spectrum of compound 7c (DMSO-*d*₆)

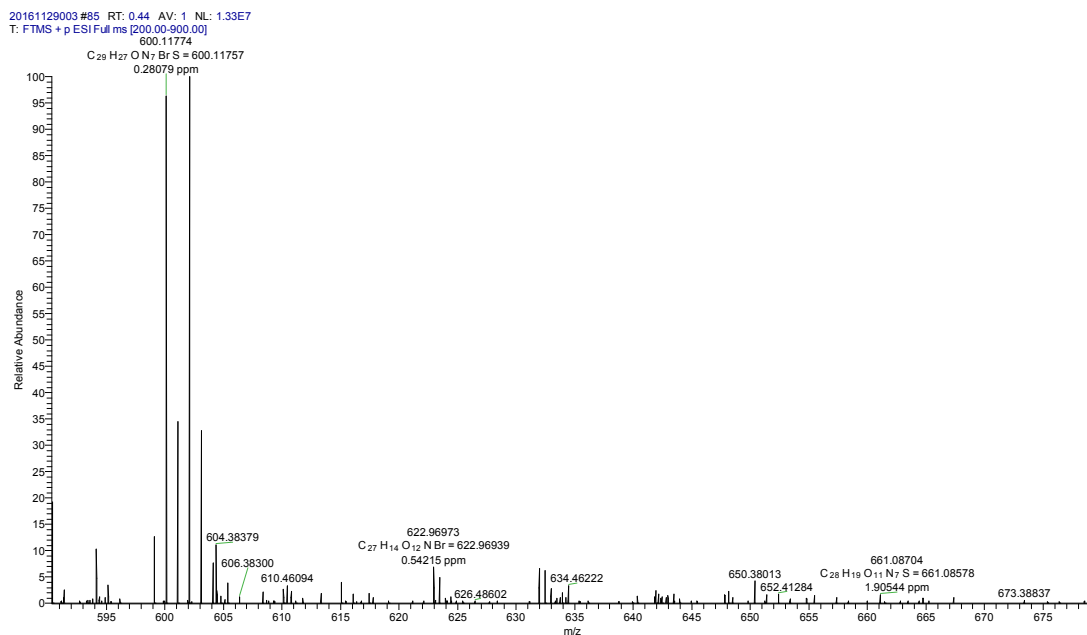


Figure S21. HRMS-ESI spectrum of compound 7c

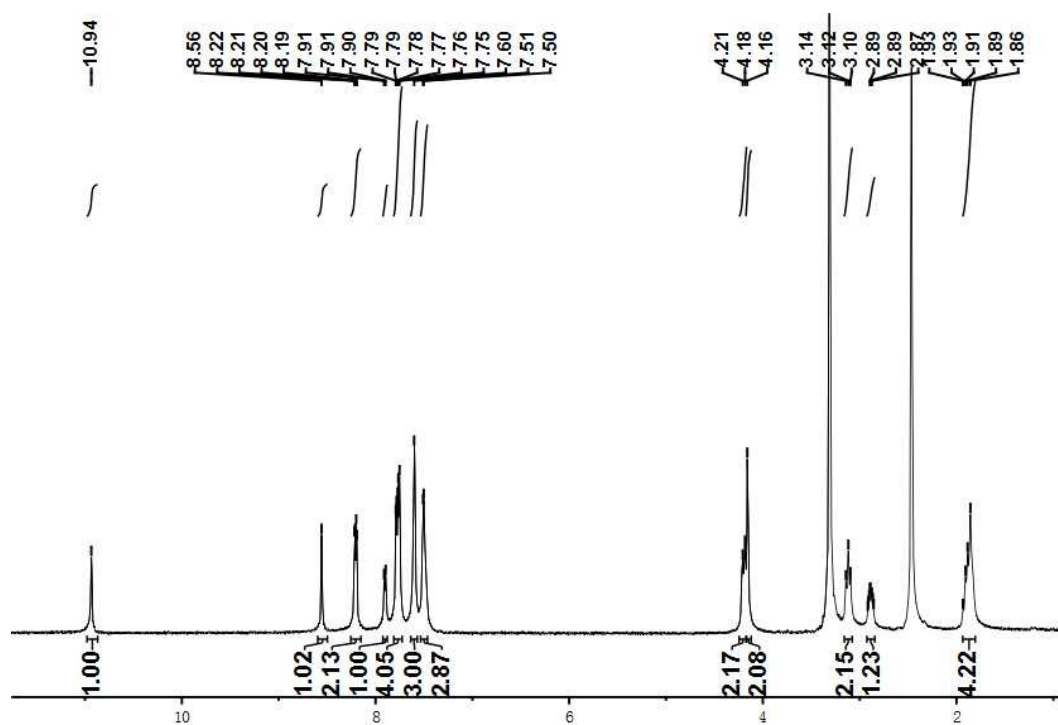


Figure S22. ¹H NMR spectrum of compound 7d (DMSO-*d*₆)

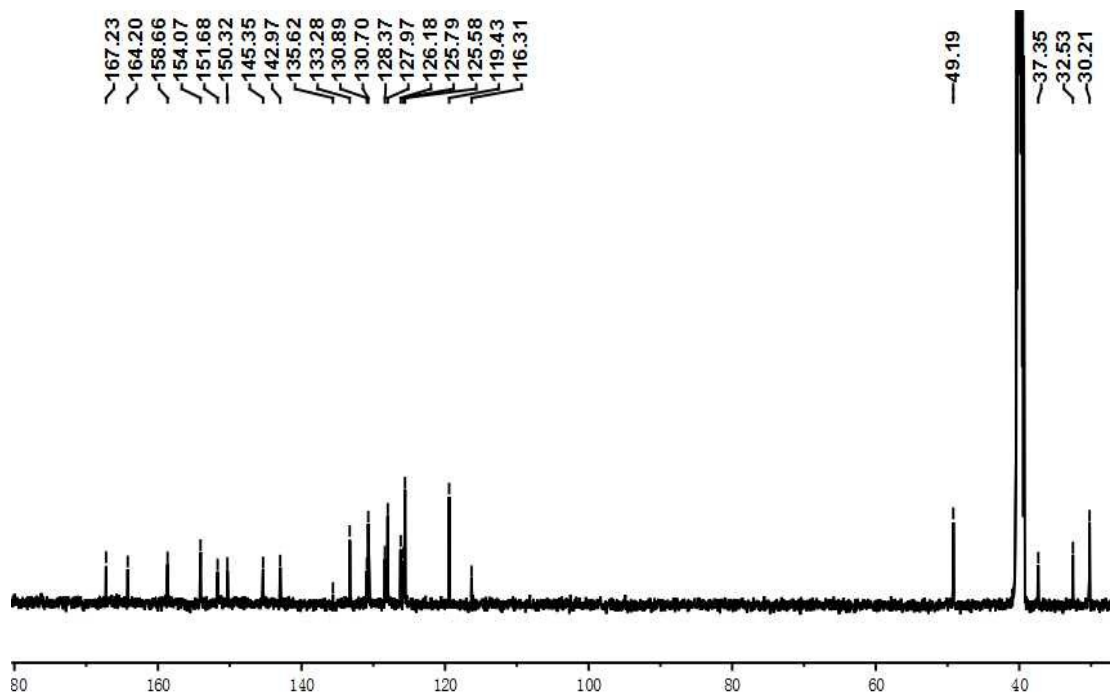


Figure S23. ^{13}C NMR spectrum of compound **7d** ($\text{DMSO}-d_6$)

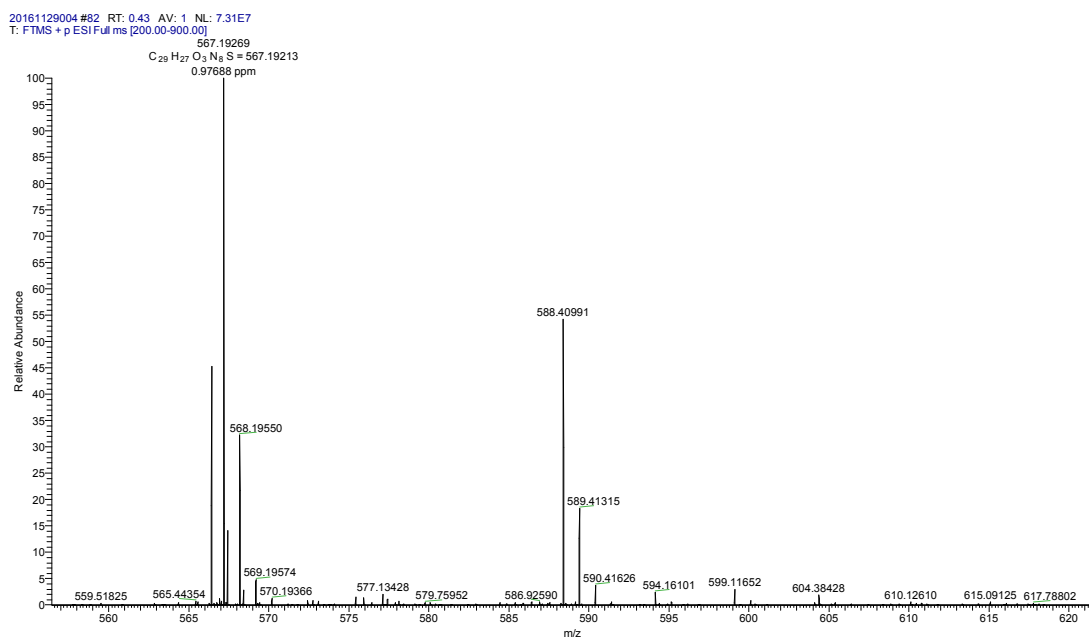


Figure S24. HRMS-ESI spectrum of compound **7d**

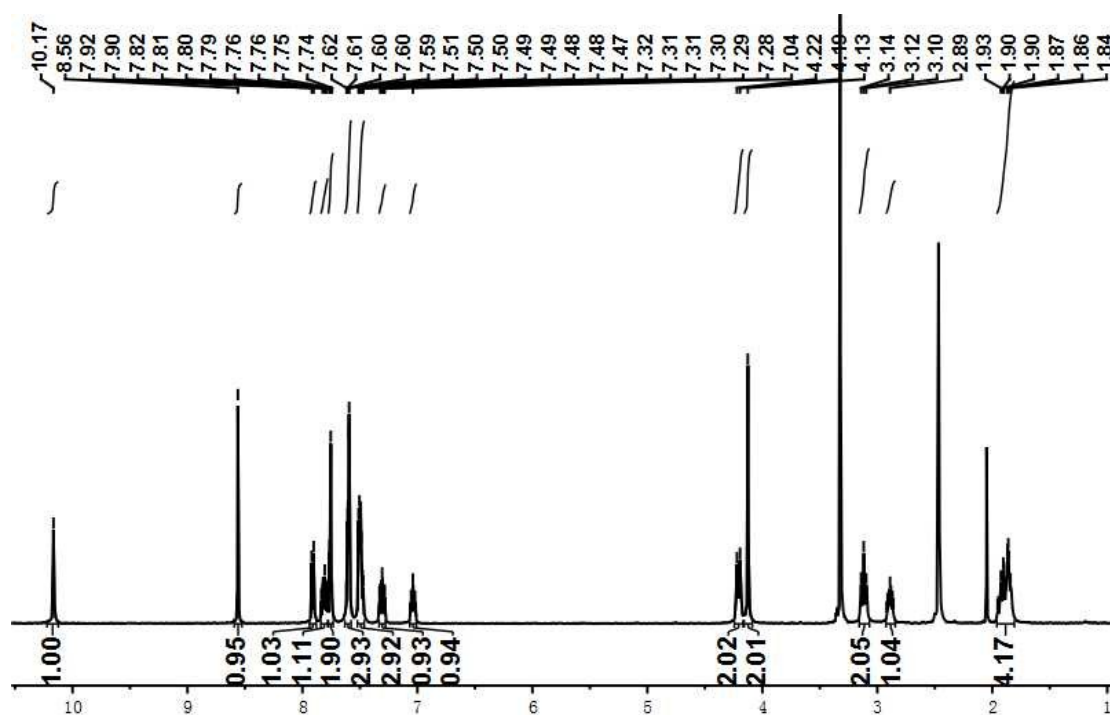


Figure S25. ^1H NMR spectrum of compound **7e** ($\text{DMSO}-d_6$)

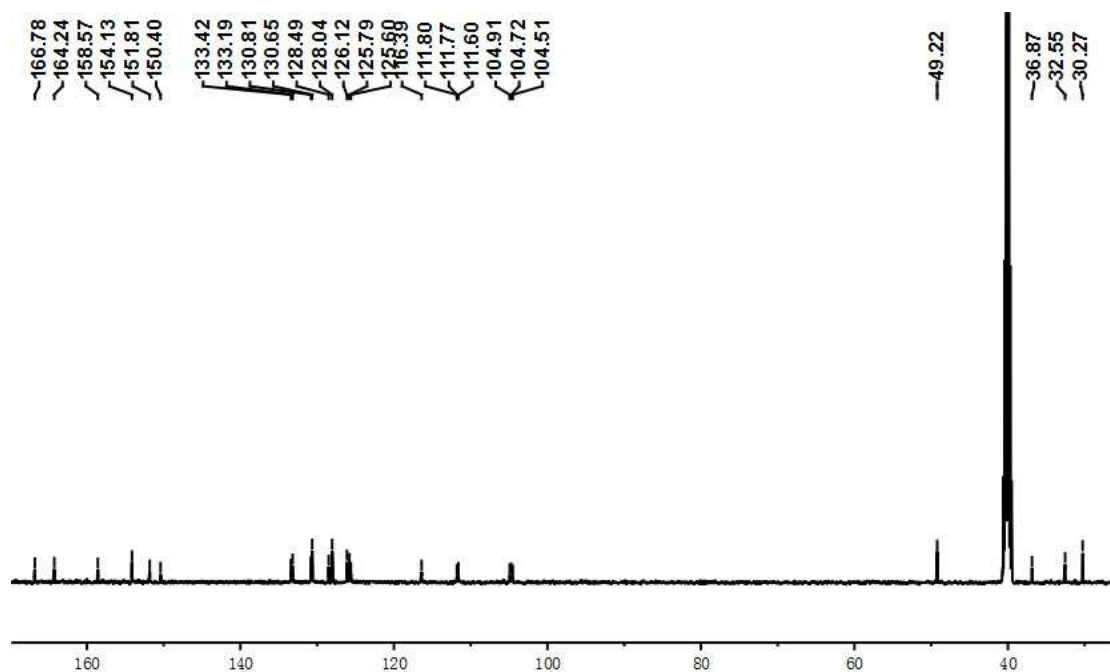


Figure S26. ^{13}C NMR spectrum of compound **7e** ($\text{DMSO}-d_6$)

20170221002_170221160215#127 RT: 0.65 AV: 1 NL: 4.96E7
T: FTMS + p ESI Full ms [200.00-800.00]

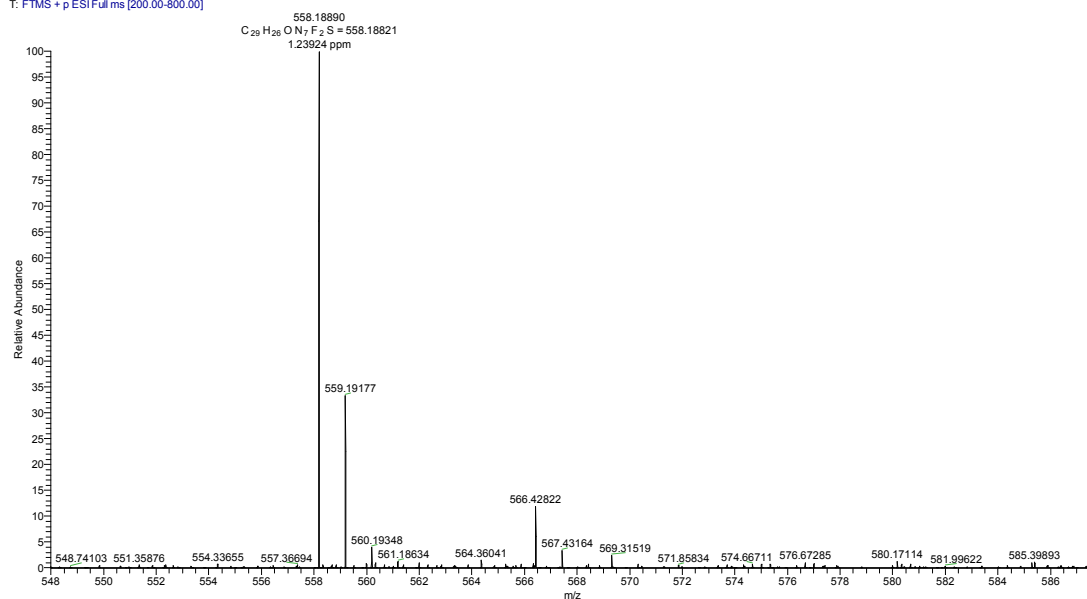


Figure S27. HRMS-ESI spectrum of compound 7e

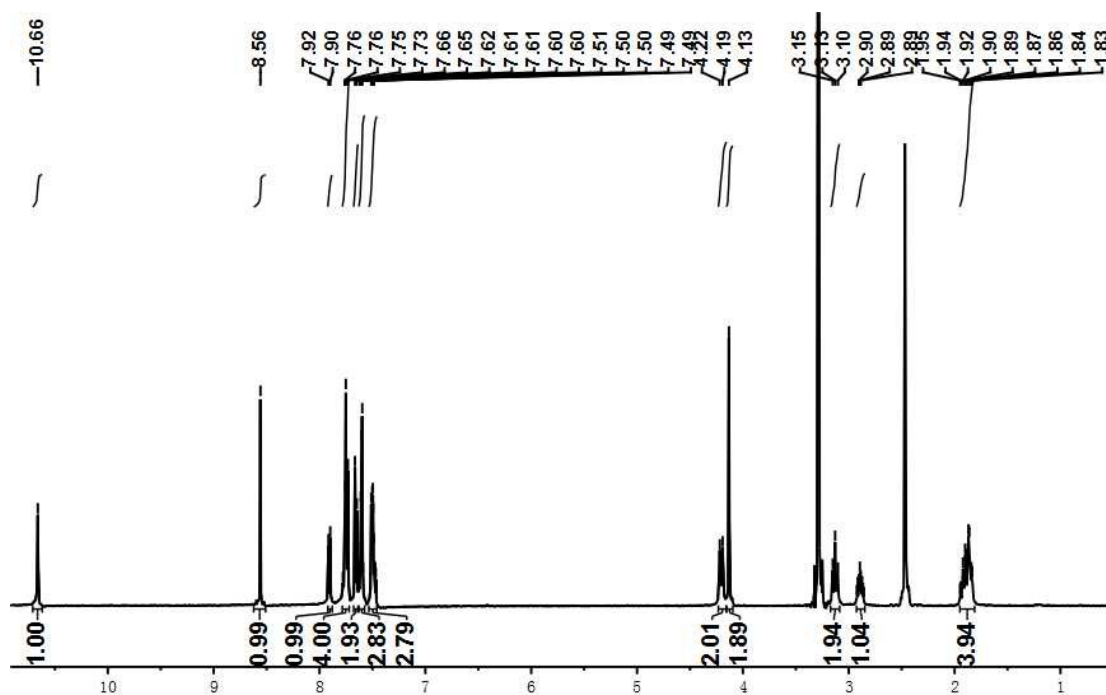


Figure S28. ¹H NMR spectrum of compound 7f (DMSO-*d*₆)

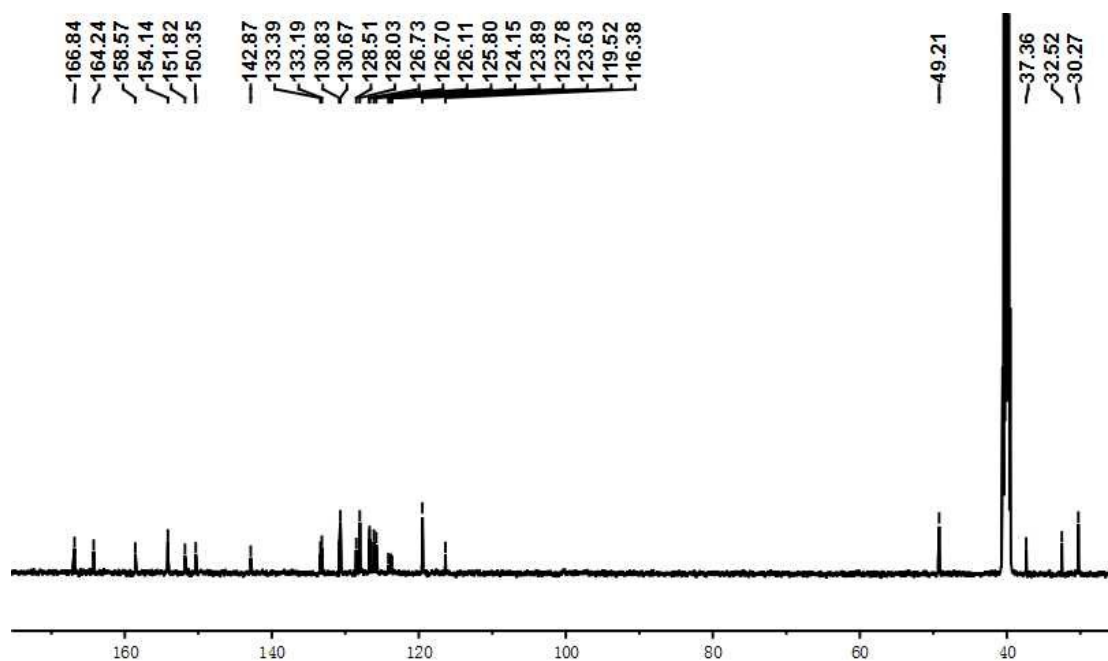


Figure S29. ^{13}C NMR spectrum of compound **7f** ($\text{DMSO}-d_6$)

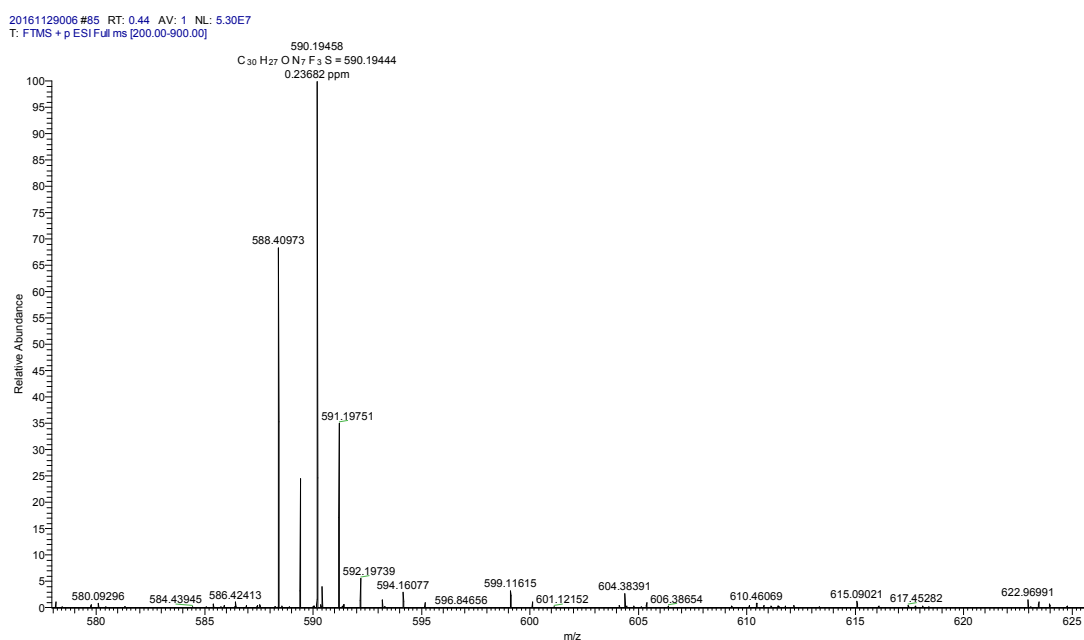


Figure S30. HRMS-ESI spectrum of compound **7f**

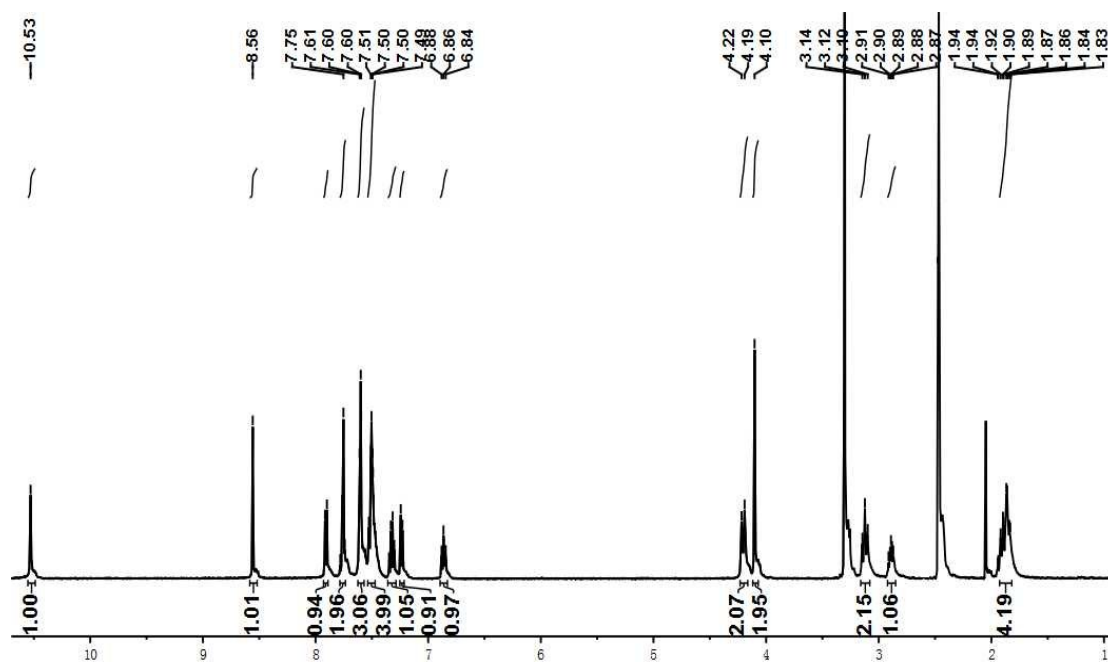


Figure S31. ¹H NMR spectrum of compound **7g** (DMSO-*d*₆)

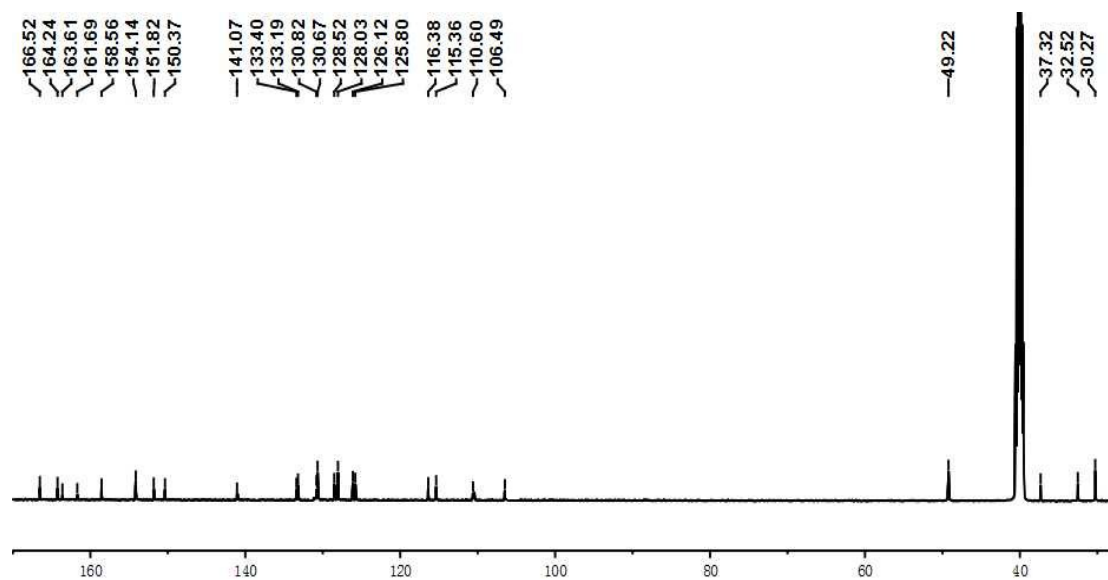


Figure S32. ¹³C NMR spectrum of compound **7g** (DMSO-*d*₆)

20161202070 #77 RT: 0.41 AV: 1 NL: 1.48E8
T: FTMS + p ESI Fullms [300.00-700.00]

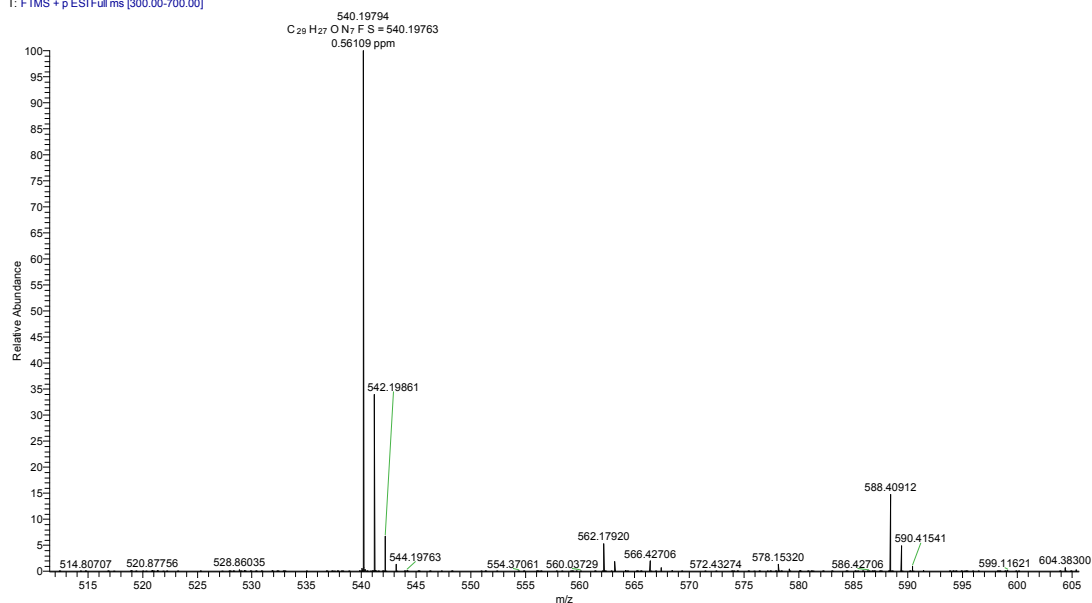


Figure S33. HRMS-ESI spectrum of compound **7g**

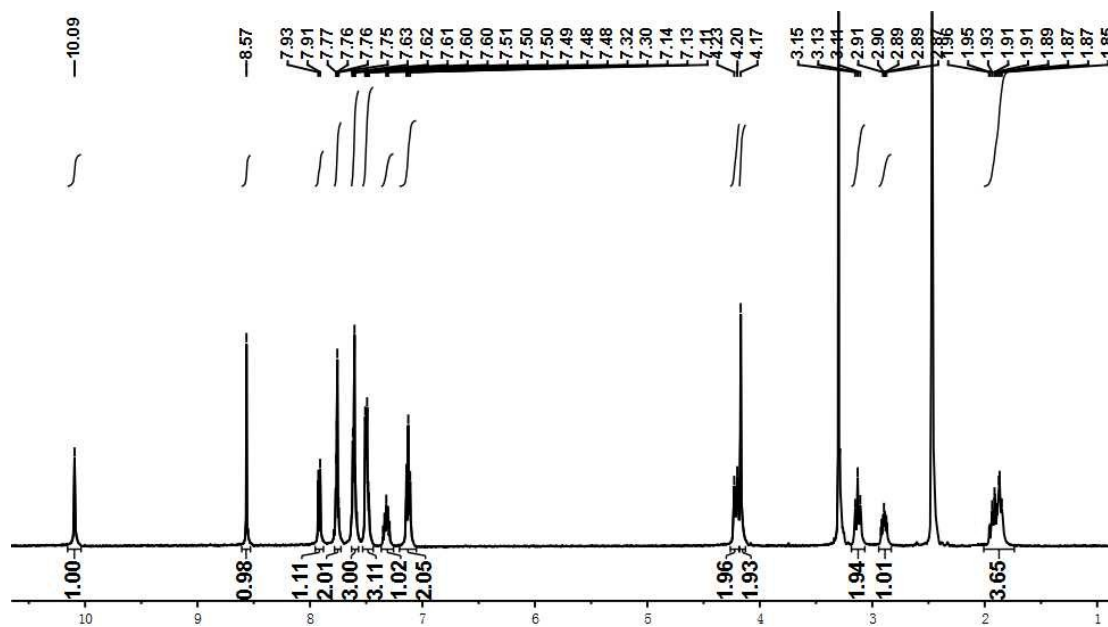


Figure S34. ¹H NMR spectrum of compound **7h** (DMSO-*d*₆)

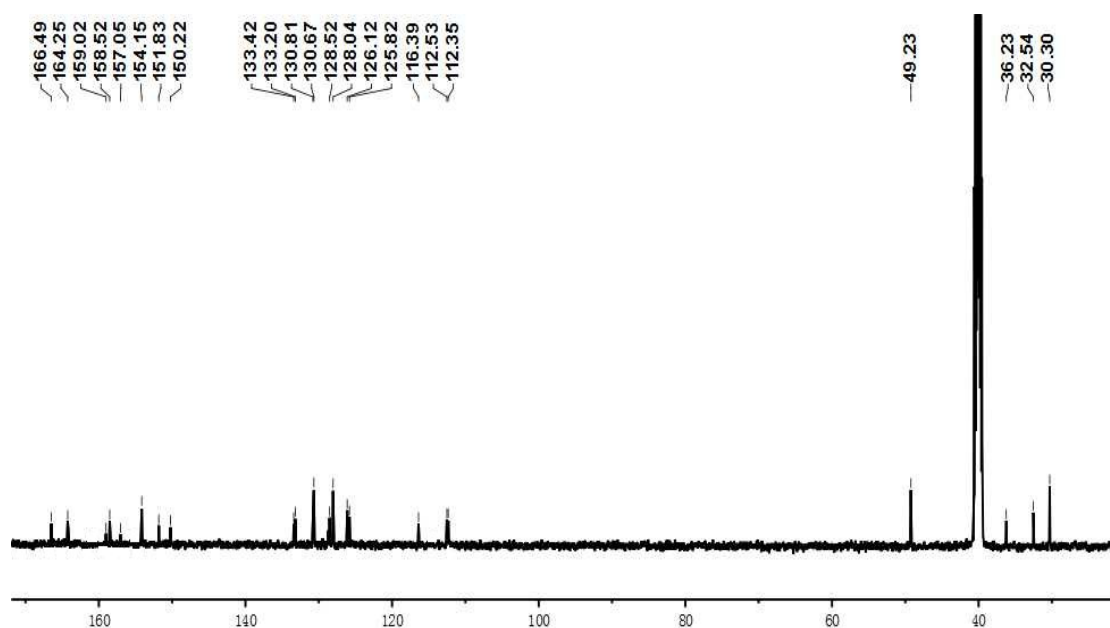


Figure S35. ^{13}C NMR spectrum of compound **7h** ($\text{DMSO}-d_6$)

20170221003 #122 RT: 0.62 AV: 1 NL: 2.19E8
T: FTMS + p ESI Full ms [200.00-800.00]

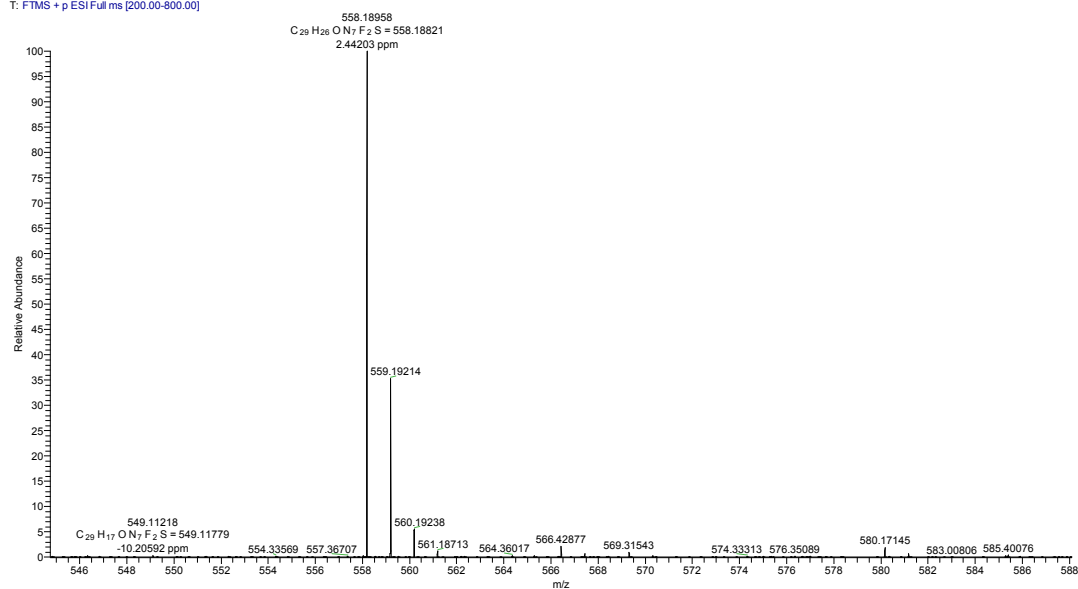


Figure S36. HRMS-ESI spectrum of compound **7h**

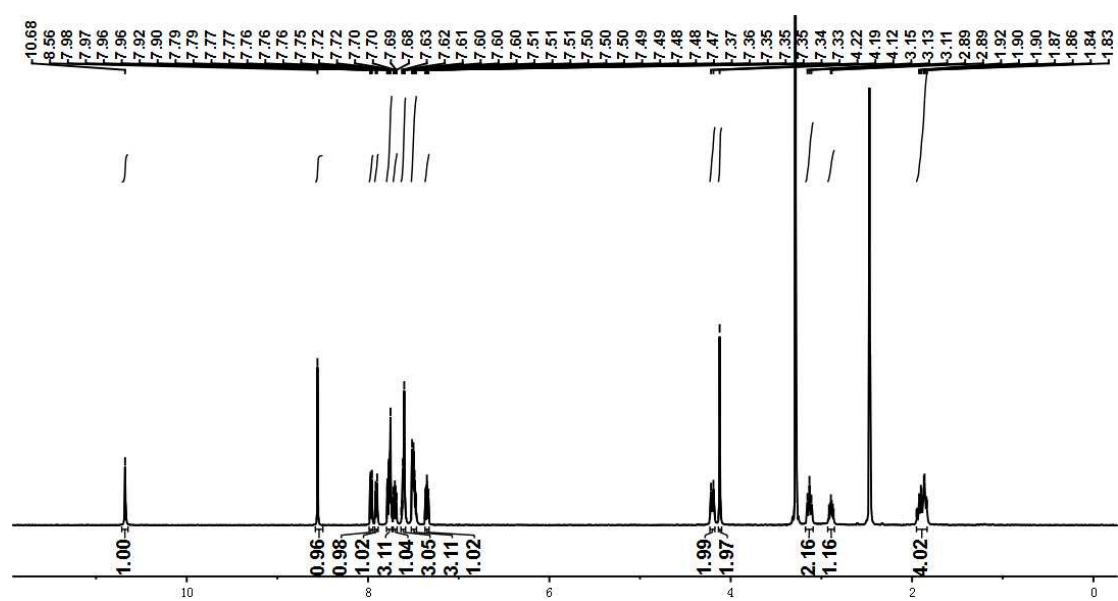


Figure S37. ^1H NMR spectrum of compound **7i** ($\text{DMSO}-d_6$)

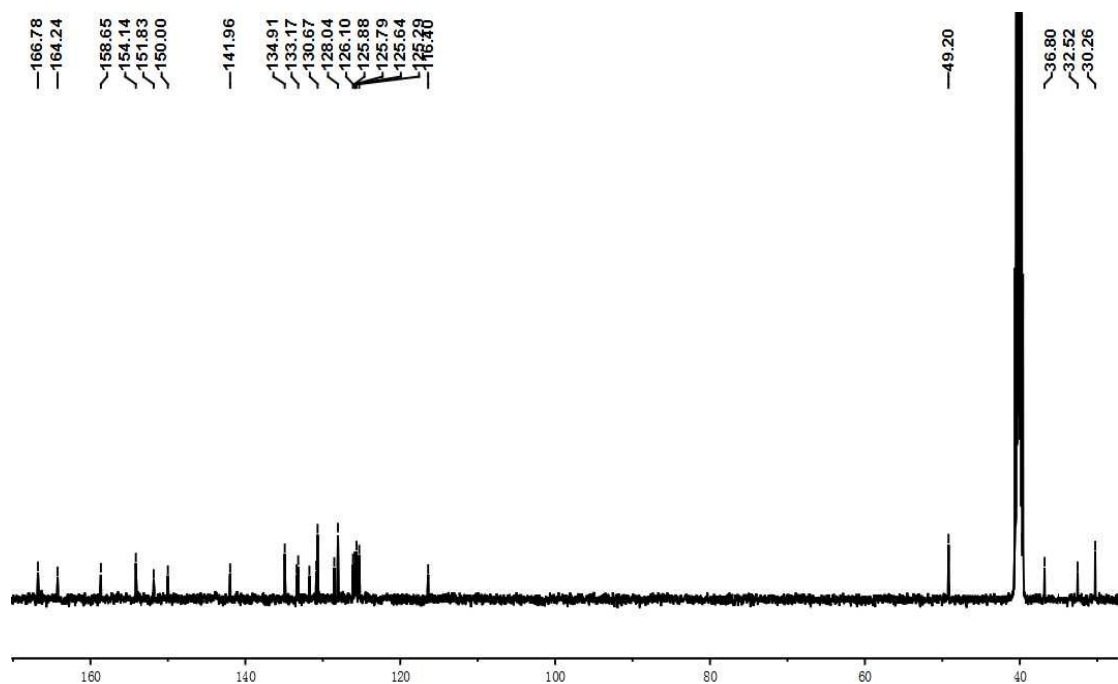


Figure S38. ^{13}C NMR spectrum of compound **7i** ($\text{DMSO}-d_6$)

20161129016 #76 RT: 0.40 AV: 1 NL: 1.07E8
T: FTMS + p ESI Full ms [200.00-900.00]

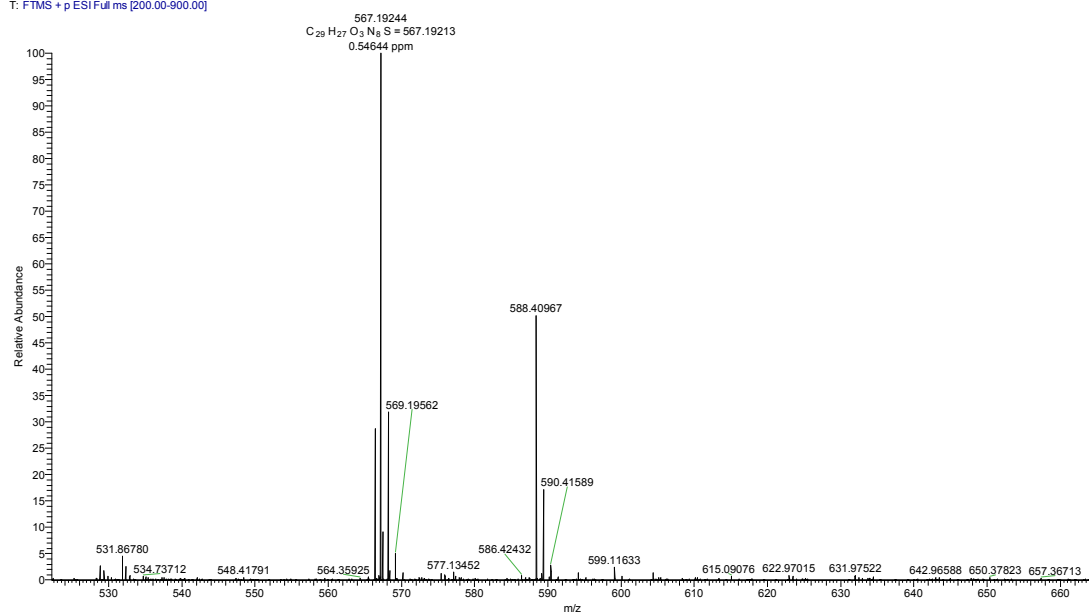


Figure S39. HRMS-ESI spectrum of compound 7i

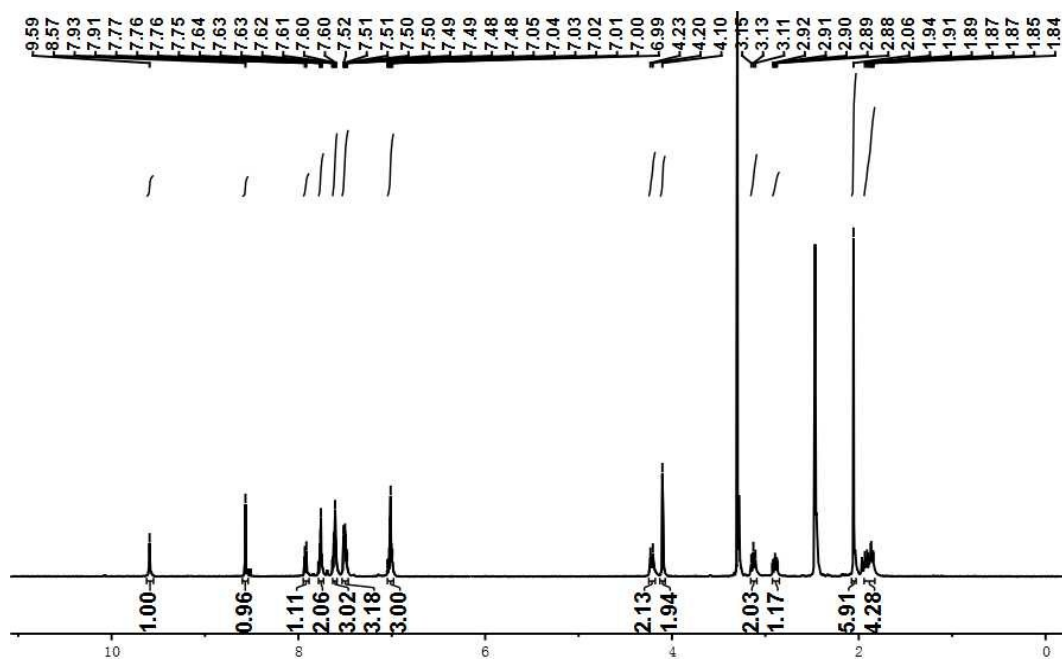


Figure S40. ¹H NMR spectrum of compound 7j (DMSO-*d*₆)

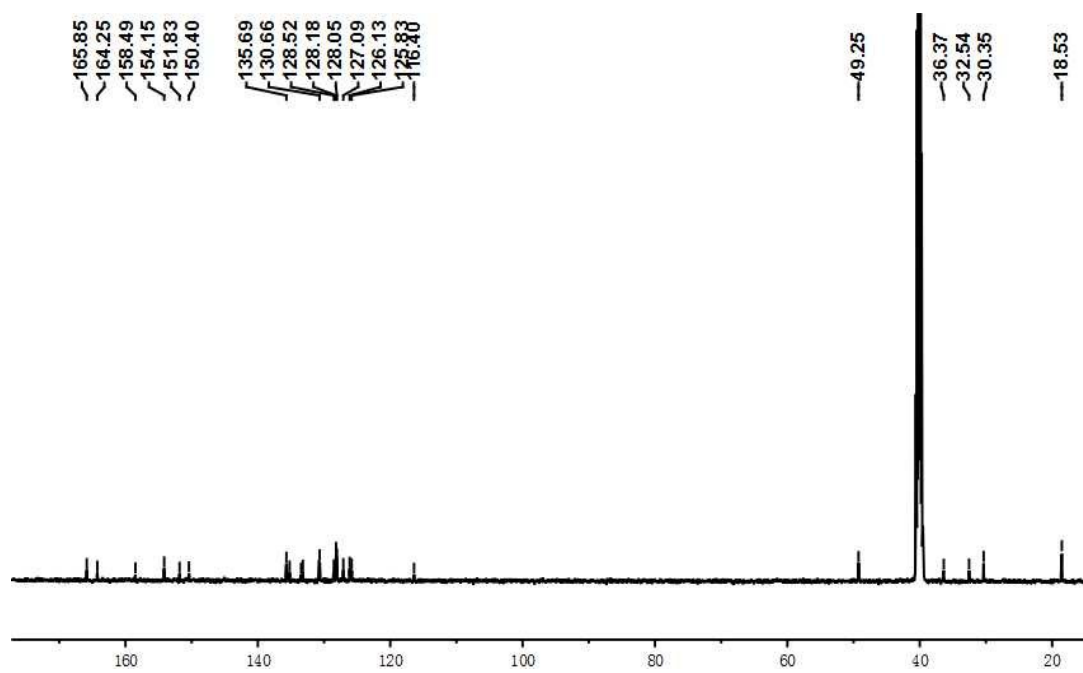


Figure S41. ^{13}C NMR spectrum of compound **7j** ($\text{DMSO}-d_6$)

20170221004 #133 RT: 0.68 AV: 1 NL: 1.96E7
T: FTMS + p ESI Full ms [200.00-800.00]

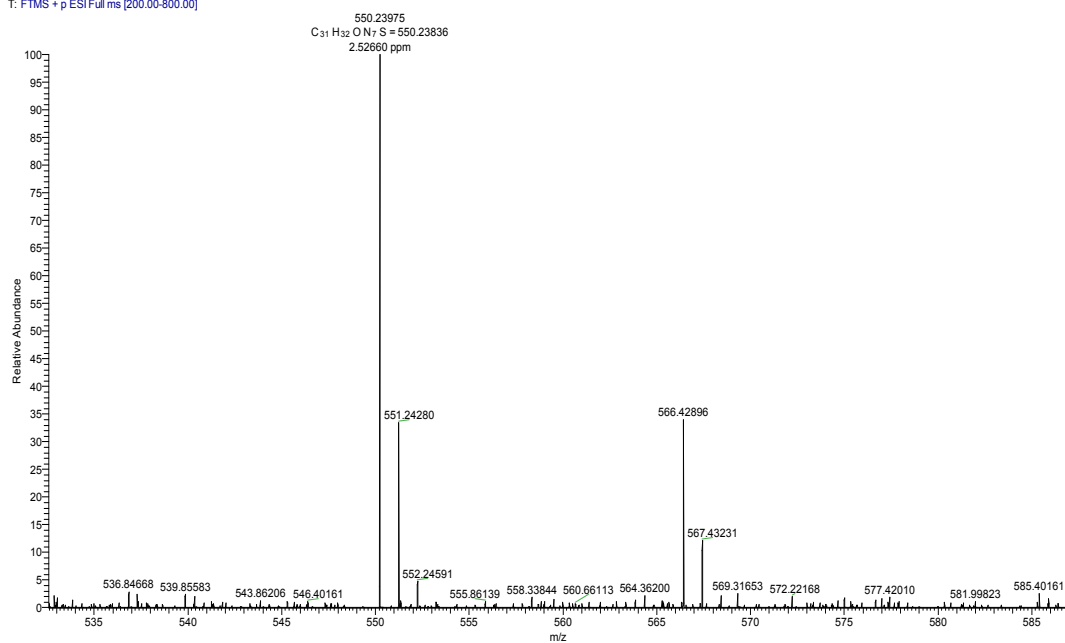


Figure S42. HRMS-ESI spectrum of compound **7j**

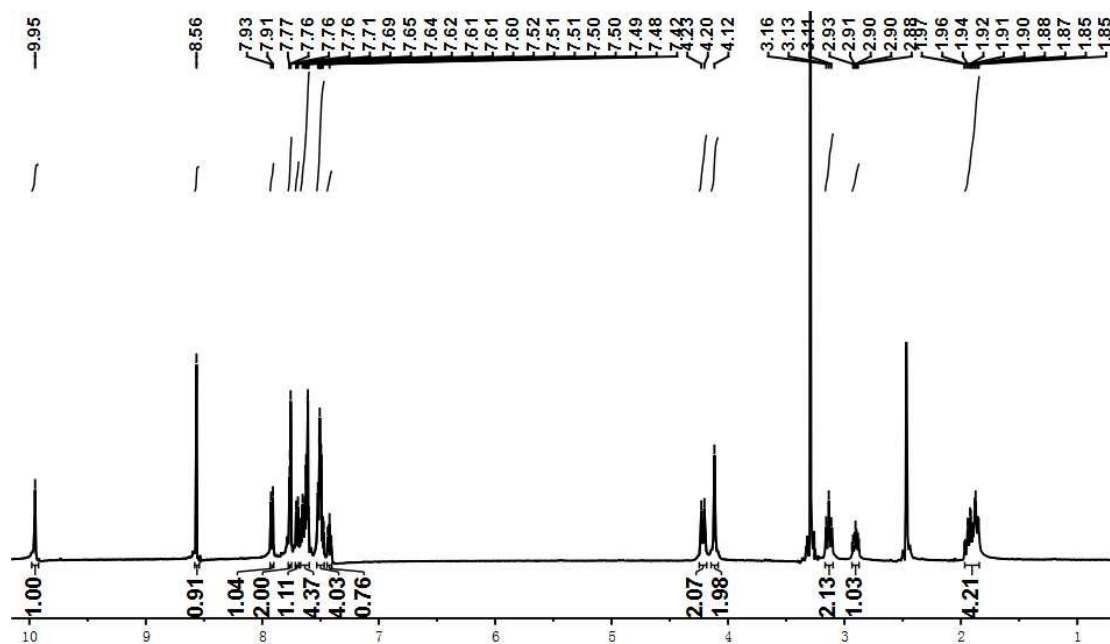


Figure S43. ¹H NMR spectrum of compound **7k** (DMSO-*d*₆)

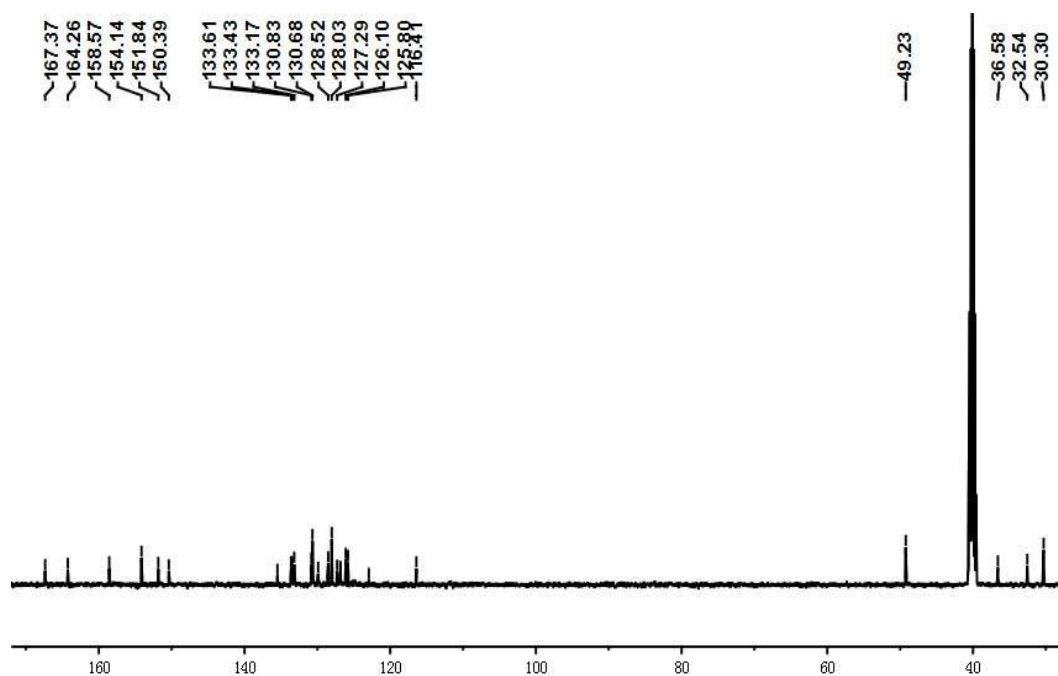


Figure S44. ¹³C NMR spectrum of compound **7k** (DMSO-*d*₆)

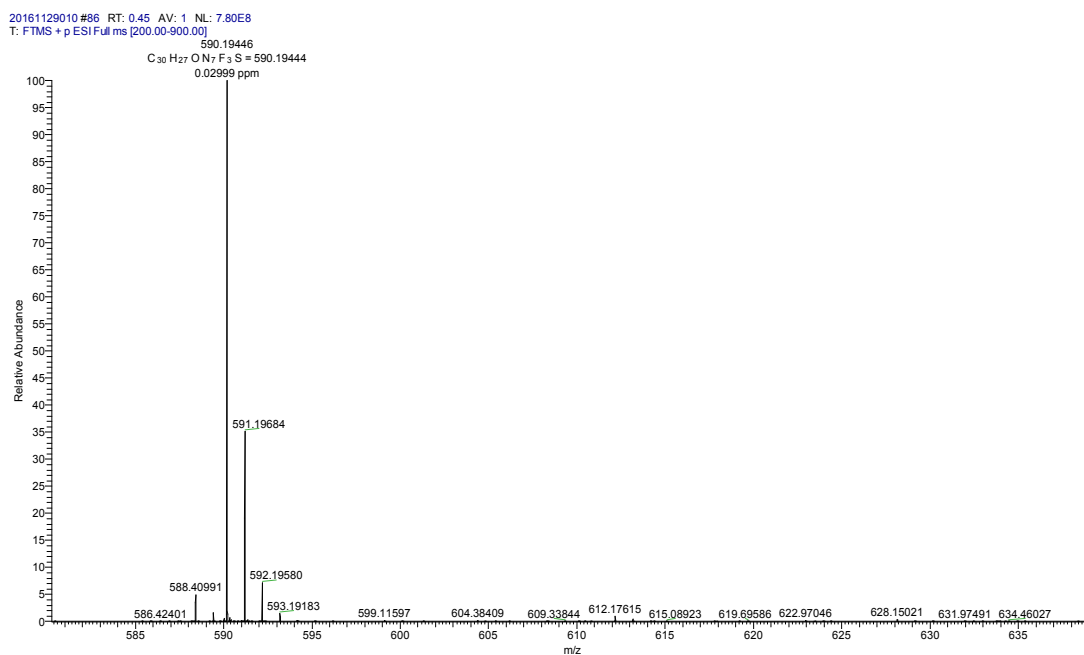


Figure S45. HRMS-ESI spectrum of compound 7k

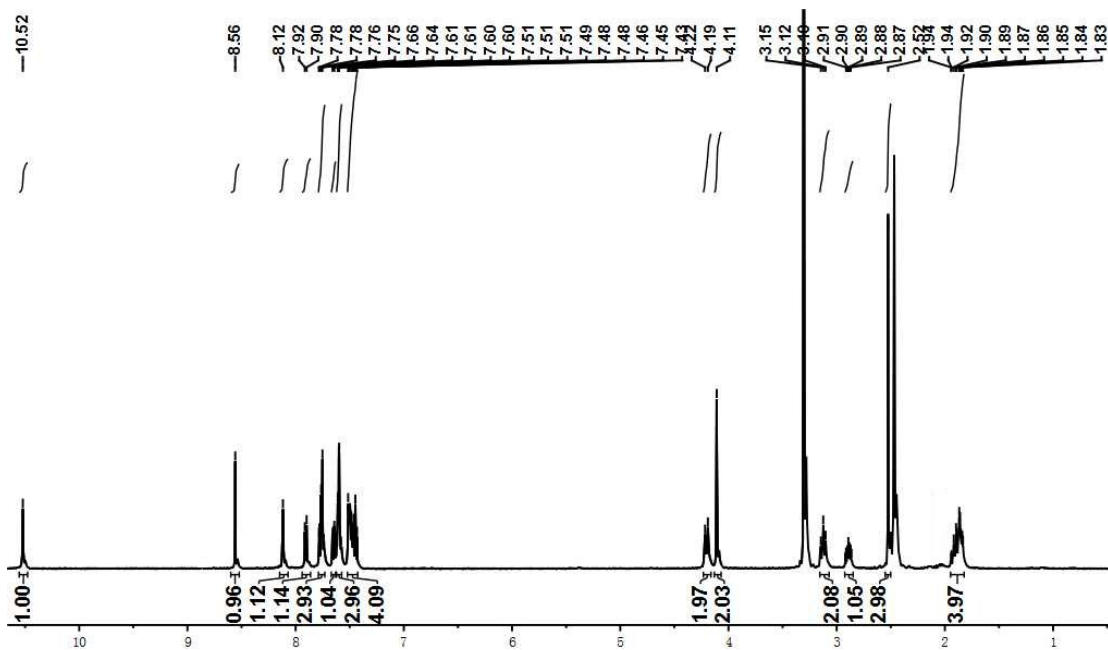


Figure S46. ^1H NMR spectrum of compound 7l ($\text{DMSO}-d_6$)

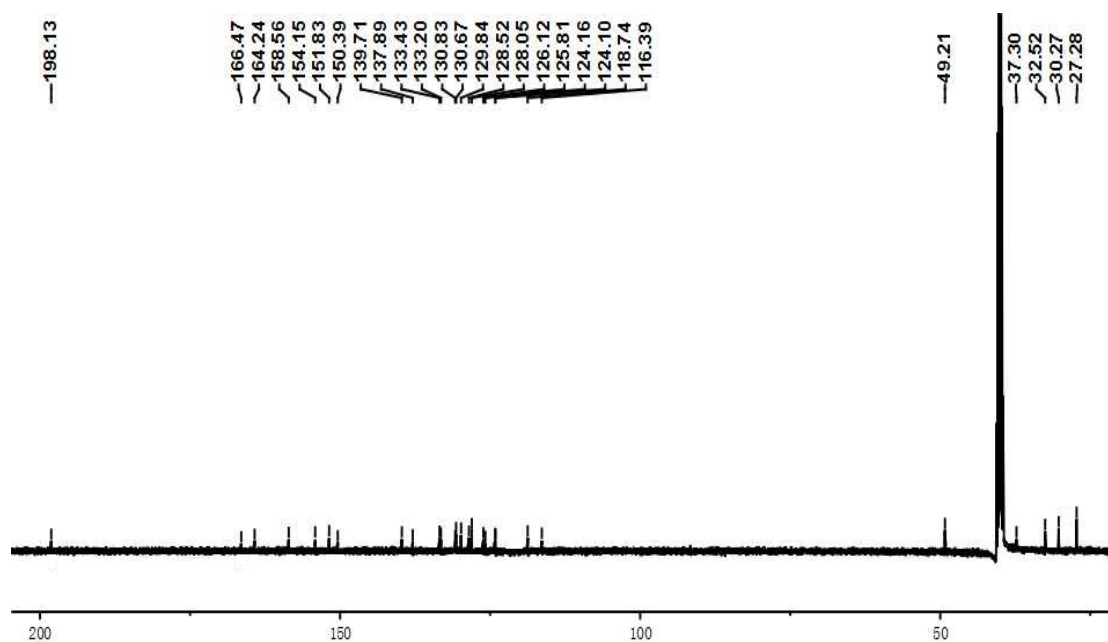


Figure S47. ¹³C NMR spectrum of compound 7I (DMSO-*d*₆)

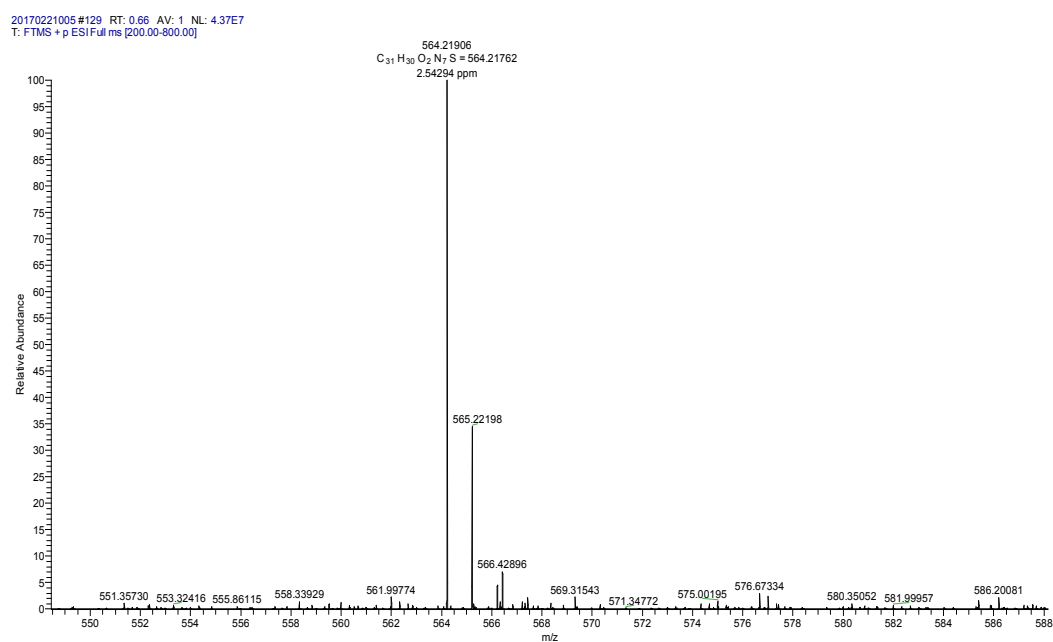


Figure S48. HRMS-ESI spectrum of compound 7I

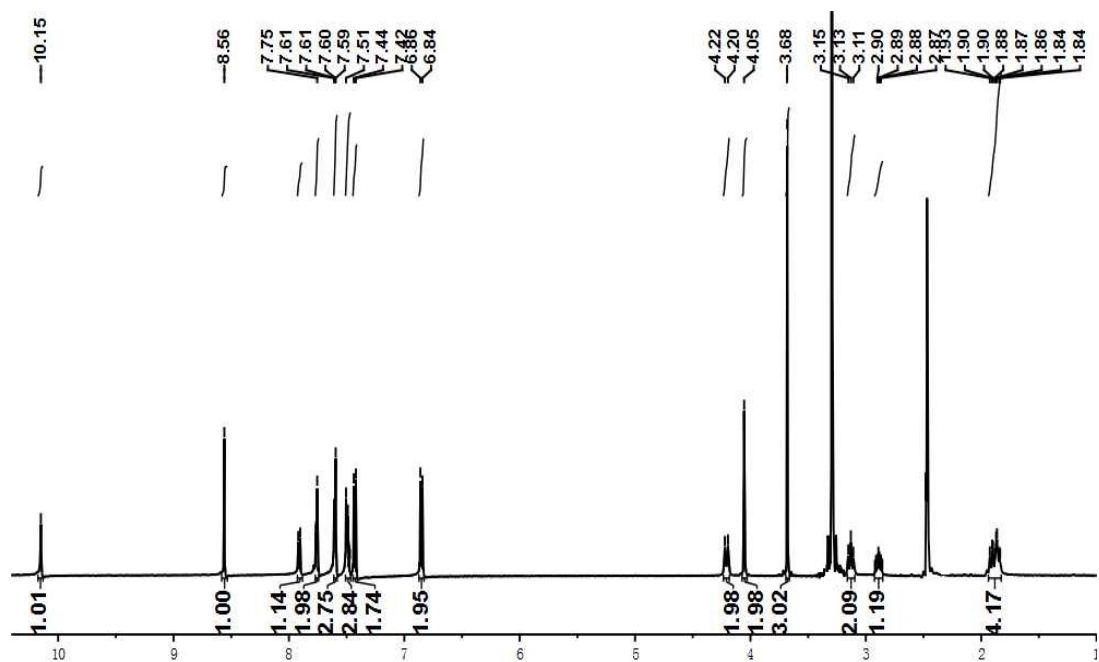


Figure S49. ¹H NMR spectrum of compound **7m** (DMSO-*d*₆)

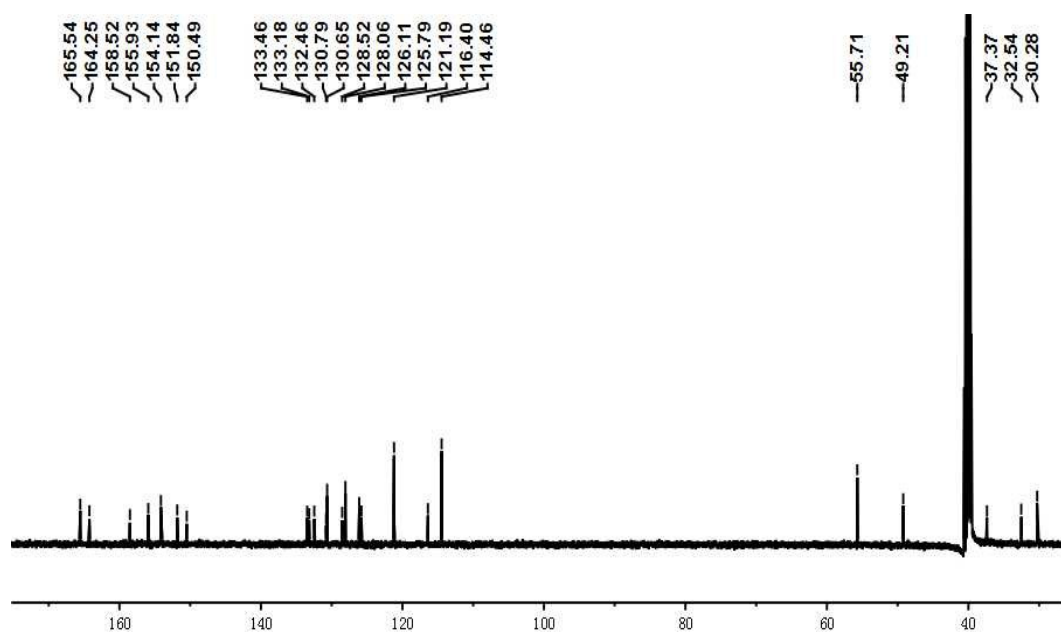


Figure S50. ¹³C NMR spectrum of compound **7m** (DMSO-*d*₆)

20170221006 #126 RT: 0.65 AV: 1 NL: 1.03E8
T: FTMS + p ESI Full ms [200.00-800.00]

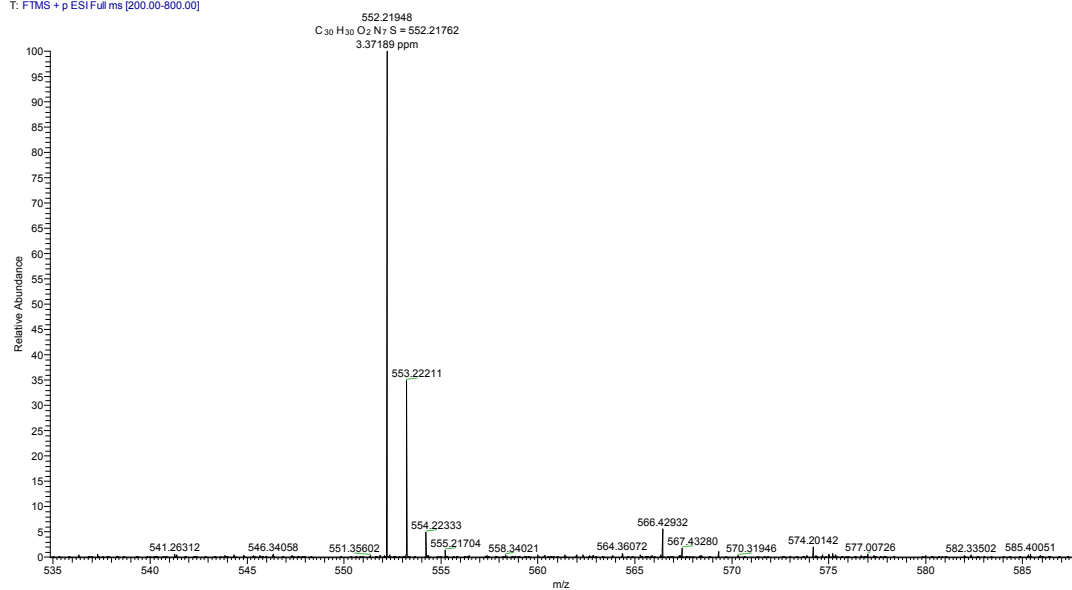


Figure S51. HRMS-ESI spectrum of compound 7m

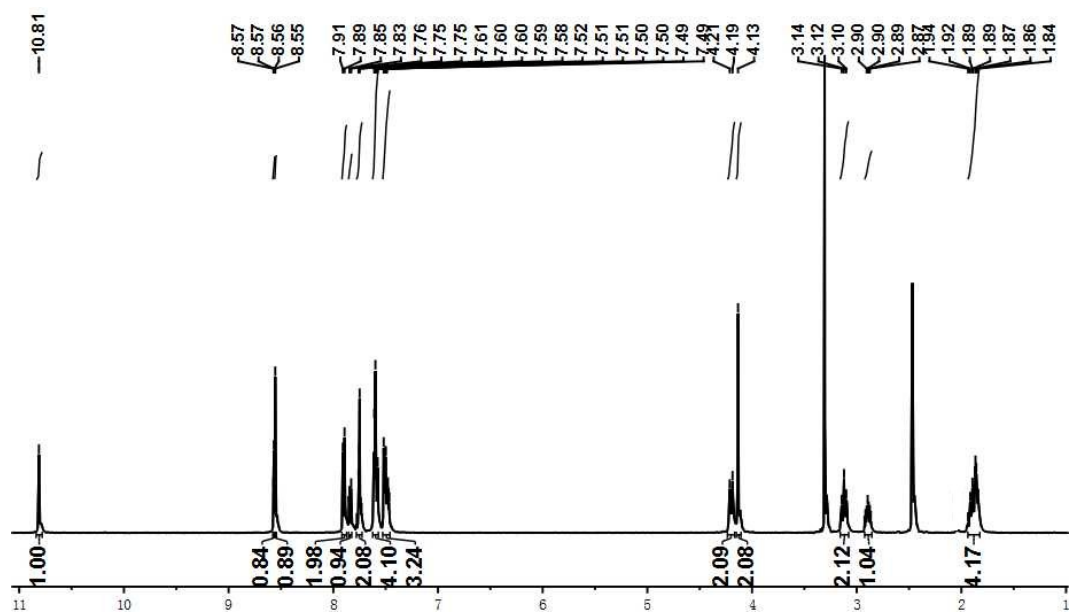


Figure S52. ¹H NMR spectrum of compound 7n (DMSO-*d*₆)

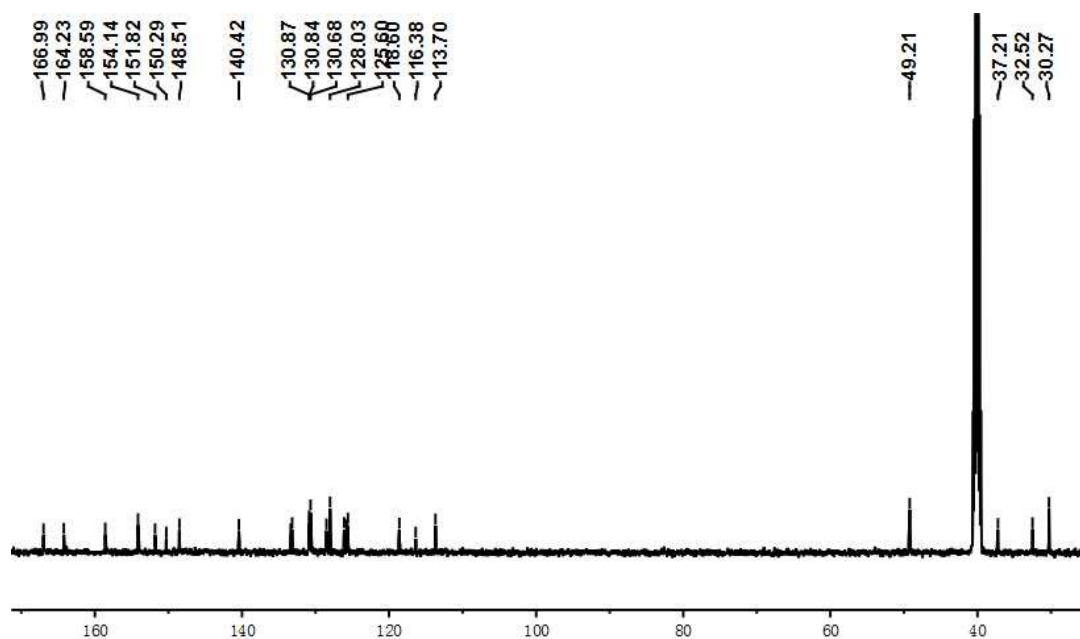


Figure S53. ^{13}C NMR spectrum of compound **7n** ($\text{DMSO}-d_6$)

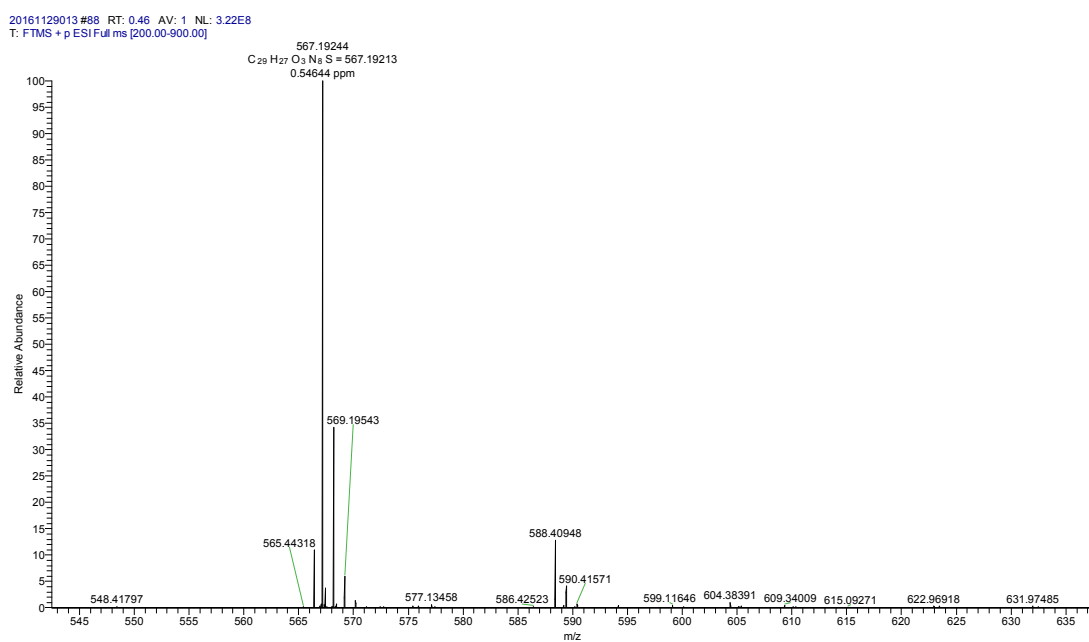
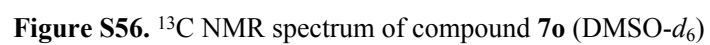
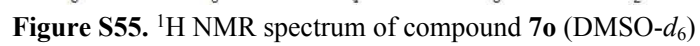


Figure S54. HRMS-ESI spectrum of compound **7n**



20170221007 #139 RT: 0.72 AV: 1 NL: 2.60E7
T: FTMS + p ESI Full ms [200.00-800.00]

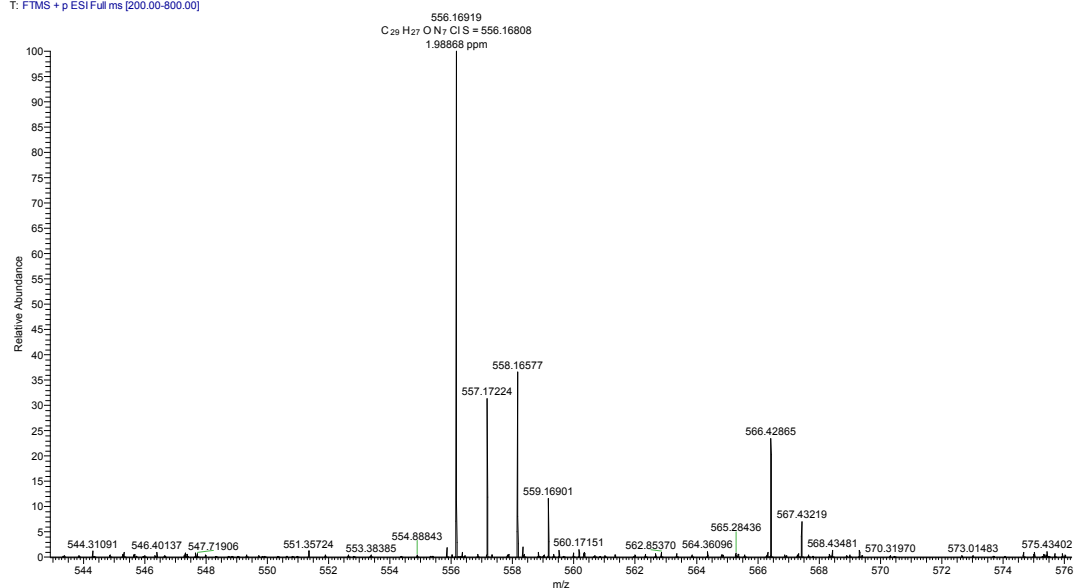


Figure S57. HRMS-ESI spectrum of compound **7o**

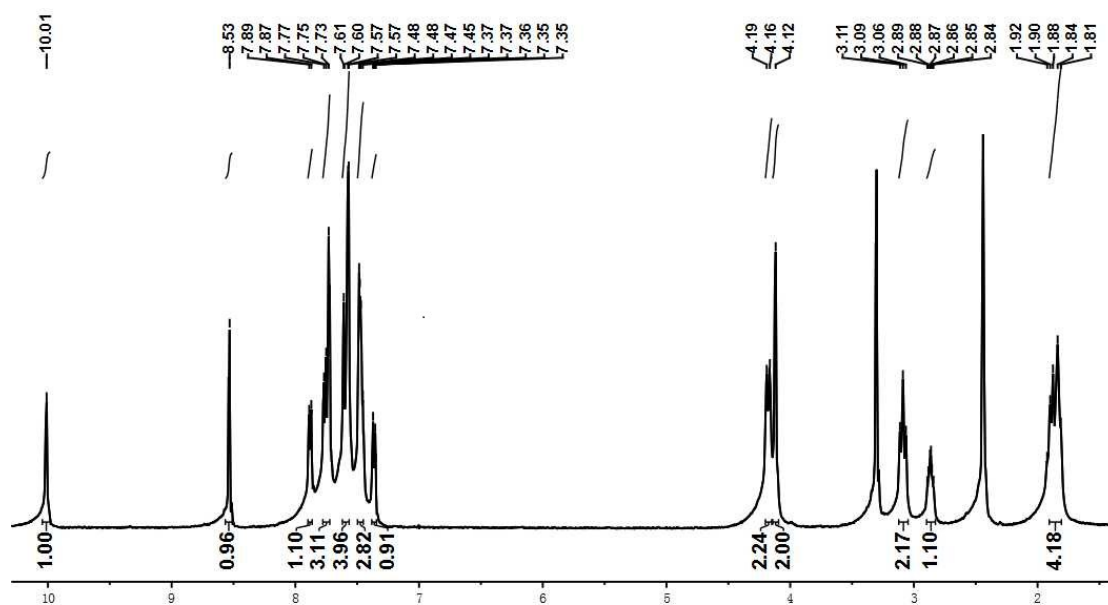


Figure S58. ¹H NMR spectrum of compound **7p** (DMSO-*d*₆)

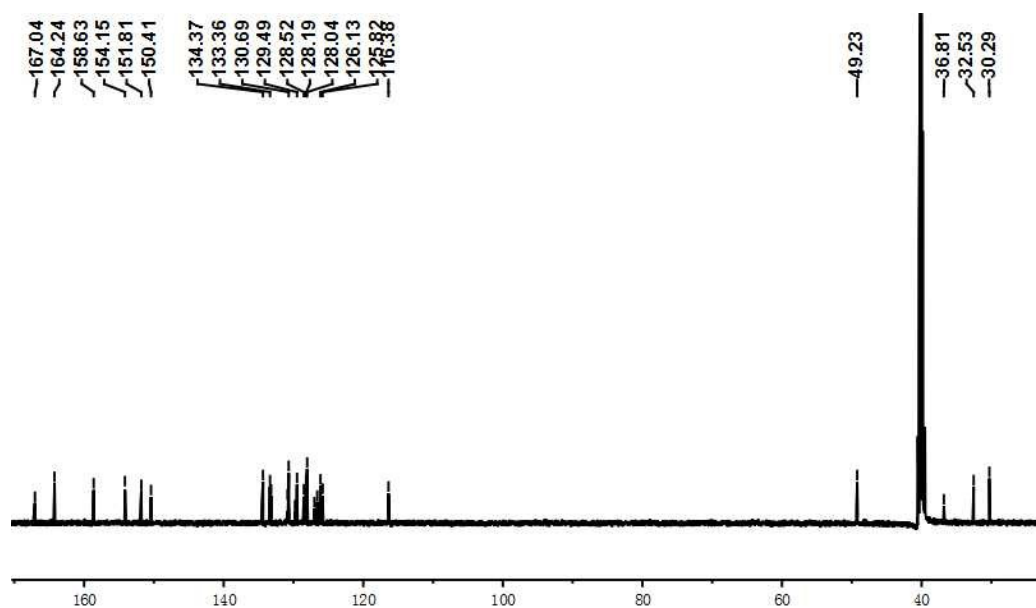


Figure S59. ^{13}C NMR spectrum of compound **7p** ($\text{DMSO}-d_6$)

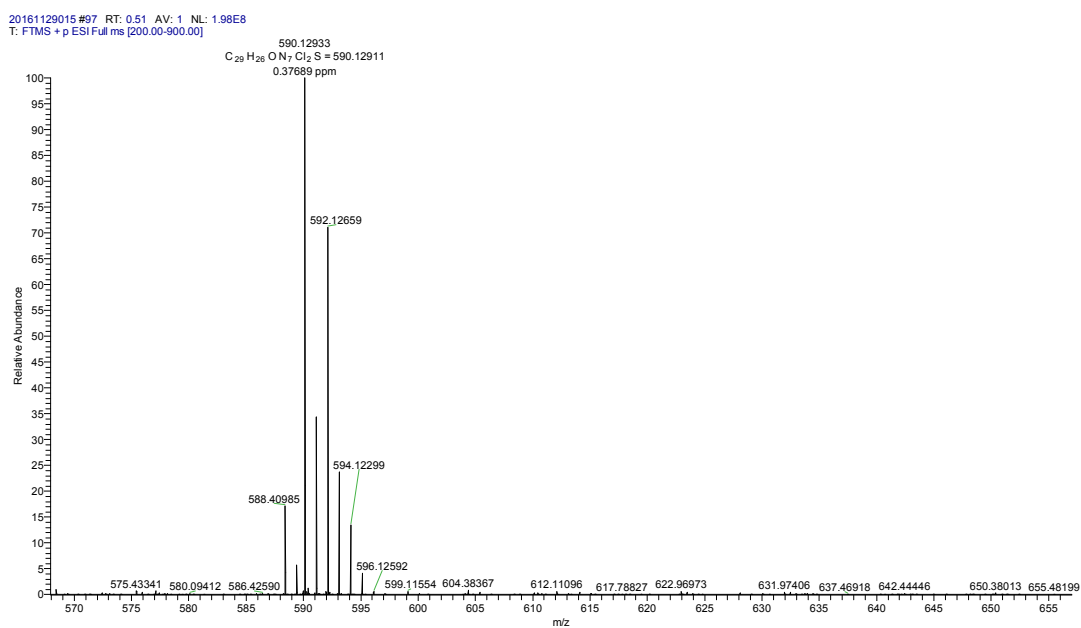


Figure S60. HRMS-ESI spectrum of compound **7p**