

Supporting Information

Development of five membered heterocyclic frameworks via [3+2] cycloaddition reaction in aqueous micellar system

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Spectral data of synthesized compounds:

Compound 4a: ¹HNMR (CDCl₃, 300MHz): δ 3.83 (s, 3H), 3.90 (s, 3H), 4.58 (s, 1H), 4.80 (s, 1H), 5.48 (d, 1H), 7.03 (d, 1H), 7.08-7.20 (m, 4H), 7.40-7.82 (m, 4H). ¹³C NMR (75 MHz) δ 52.03, 53.01, 66.68, 67.68, 98.52, 126.31, 126.24, 127.31, 127.82, 128.4, 129.4, 129.78, 130.64, 131.44, 132.4, 133.83, 134.99, 137.54, 138.28, 140.53, 168.43, 169.19, 195.49. Anal. Calcd. For C₂₃H₁₈ClNO₅: C, 65.18; H, 4.28; N, 3.30; found C, 65.12; H, 4.20; N, 3.28.

Compound 4b: ¹HNMR (CDCl₃, 300MHz): δ 3.84 (s, 3H), 3.90 (s, 3H), 4.57 (s, 1H), 4.80 (s, 1H), 5.47 (d, 1H), 7.00 (d, 1H), 7.06-7.18 (m, 4H), 7.29-7.40 (m, 4H). ¹³C NMR (75 MHz) δ 52.06, 53.04, 66.68, 67.25, 98.52, 126.24, 126.31, 126.88, 127.31, 127.82, 128.48, 129.78, 130.49, 131.91, 132.44, 133.83, 135.99, 137.54, 137.86, 138.28, 168.43, 169.19, 194.83. Anal. Calcd. For C₂₃H₁₈ClNO₅: C, 65.18; H, 4.28; N, 3.30; found C, 65.16; H, 4.28; N, 3.26.

Compound 4c: ¹HNMR (CDCl₃, 300MHz): δ 3.83 (s, 3H), 3.85 (s, 3H), 3.89 (s, 3H), 4.60 (s, 1H), 4.79 (s, 1H), 5.46 (d, 1H), 7.02-7.20 (m, 7H), 7.80 (m, 2H). ¹³C NMR (75 MHz) δ 52.04, 53.08, 56.04, 66.68, 67.68, 98.52, 113.69, 114.72, 126.24, 126.31, 127.31, 127.82, 129.78, 130.98, 131.43, 131.92, 132.44, 133.83, 137.54, 138.28, 163.75, 168.43, 169.19, 195.39. Anal. Calcd. For C₂₄H₂₁NO₆: C, 68.73; H, 5.05; N, 3.34; found C, 68.67; H, 5.00; N, 3.30.

Compound 4d: ¹HNMR (CDCl₃, 300MHz): δ 3.84 (s, 3H), 3.92 (s, 3H), 4.60 (s, 1H), 4.80 (s, 1H), 5.40 (s, 1H), 5.62 (d, 1H), 6.82 (d, 1H), 6.99 (m, 2H), 7.05-7.40 (m, 6H). ¹³C NMR (75 MHz) δ 52.12, 53.03, 66.68, 67.25, 98.52, 119.22, 119.65, 121.49, 126.24, 126.31, 127.31, 127.82, 129.78, 130.61, 132.44, 133.83, 134.96, 137.54, 138.28, 162.37, 168.43, 169.19, 200.09. Anal. Calcd. For C₂₃H₁₉NO₆: C, 68.14; H, 4.72; N, 3.46; found C, 68.14; H, 4.70; N, 3.38.

Compound 4e: ¹HNMR (CDCl₃, 300MHz): δ 3.80 (s, 3H), 3.87 (s, 3H), 3.90 (s, 3H), 4.60 (s, 1H), 4.80 (s, 1H), 5.38 (s, 1H), 5.48 (d, 1H), 6.81 (d, 1H), 7.05 (m, 1H), 7.12-7.38 (m, 6H). ¹³C NMR (75 MHz) δ 52.01, 53.07, 56.79, 66.68, 67.68, 98.52, 111.88, 113.98, 122.64, 126.24, 126.51, 127.31, 127.82, 129.78, 131.22, 132.44, 133.83, 137.54, 138.28, 146.61, 153.48, 168.43, 169.19, 193.54. Anal. Calcd. For C₂₄H₂₁NO₇: C, 66.20; H, 4.86; N, 3.22; found C, 66.18; H, 4.78; N, 3.14.

Compound 4f: ¹HNMR (CDCl₃, 300MHz): δ 3.83 (s, 3H), 3.90 (s, 3H), 4.58 (s, 1H), 4.80 (s, 1H), 5.50 (d, 1H), 7.02 (d, 1H), 7.08-7.20 (m, 4H), 8.08 (m, 4H). ¹³C NMR (75 MHz) δ 53.03, 66.68, 67.68, 98.52, 123.76, 124.76, 126.24, 126.51, 127.31, 127.82, 129.58, 130.28,

131.68, 132.44, 133.83, 137.54, 138.28, 143.65, 149.73, 168.43, 169.19, 195.59. Anal. Calcd. For C₂₃H₁₈N₂O₇: C, 63.59; H, 4.18; N, 6.45; found C, 63.51; H, 4.12; N, 6.43.

Compound 4g: ¹HNMR (CDCl₃, 300MHz): δ 1.35 (t, 3H), 1.40 (t, 3H), 4.20 (q, 2H), 4.27 (q, 2H), 4.60 (s, 1H), 4.80 (s, 1H), 5.48 (d, 1H), 7.06 (d, 1H), 7.11-7.35 (m, 6H), 7.65-7.72 (m, 2H). ¹³C NMR (75 MHz) δ 14.7, 18.54, 61.5, 62.2, 66.68, 67.68, 98.52, 126.04, 126.31, 127.31, 127.82, 129.04, 129.34, 129.78, 130.64, 131.64, 132.44, 134.99, 135.18, 137.54, 139.27, 140.53, 165.71, 167.12, 195.67. Anal. Calcd. For C₂₅H₂₂ClNO₅: C, 66.45; H, 4.91; N, 3.10; found C, 66.39; H, 4.90; N, 3.08.

Compound 4h: ¹HNMR (CDCl₃, 300MHz): δ 1.28 (t, 3H), 1.39 (t, 3H), 3.81 (s, 3H), 4.20 (q, 2H), 4.25 (q, 2H), 4.60 (s, 1H), 4.81 (s, 1H), 5.38 (d, 1H), 7.00 (d, 1H), 7.04-7.18 (m, 6H), 7.82-7.88 (m, 2H). ¹³C NMR (75 MHz) δ 14.17, 18.68, 56.04, 61.82, 63.01, 66.68, 67.68, 98.52, 113.69, 114.63, 126.24, 126.31, 127.31, 127.82, 129.78, 130.98, 131.14, 131.73, 132.44, 135.18, 137.54, 139.27, 163.75, 165.71, 167.12, 195.45. Anal. Calcd. For C₂₆H₂₅NO₆: C, 69.79; H, 5.63; N, 3.13; found C, 69.77; H, 5.55; N, 3.13.

Compound 4i: ¹HNMR (CDCl₃, 300MHz): δ 1.38 (t, 3H), 1.43 (t, 3H), 4.19 (q, 2H), 4.25 (q, 2H), 4.60 (s, 1H), 4.81 (s, 1H), 5.59 (d, 1H), 6.90 (d, 1H), 7.15-7.30 (m, 4H), 7.95-8.20 (m, 4H). ¹³C NMR (75 MHz) δ 14.64, 18.94, 61.48, 62.5, 66.68, 67.68, 98.52, 123.76, 124.66, 126.24, 126.71, 127.31, 127.82, 129.28, 129.98, 130.78, 132.44, 135.18, 137.54, 139.27, 143.65, 149.73, 165.71, 167.12, 195.47. Anal. Calcd. For C₂₅H₂₂N₂O₇: C, 64.93; H, 4.80; N, 6.06; found C, 64.93; H, 4.78; N, 6.02.

Compound 4j: ¹HNMR (CDCl₃, 300MHz): δ 1.38 (t, 3H), 1.47 (t, 3H), 4.20 (q, 2H), 4.25 (q, 2H), 4.59 (s, 1H), 4.81 (s, 1H), 5.40 (d, 1H), 6.86-7.00 (m, 3H), 7.04-7.30 (m, 5H), 7.70-7.74 (m, 1H). ¹³C NMR (75 MHz) δ 63.08, 66.68, 67.25, 98.52, 119.22, 119.65, 121.49, 126.24, 126.61, 127.31, 127.82, 129.78, 130.61, 132.44, 134.96, 135.18, 137.54, 139.27, 162.37, 165.71, 167.12, 200.09. Anal. Calcd. For C₂₅H₂₃NO₆: Elemental Analysis: C, 69.27; H, 5.35; N, 3.23; found C, 69.23; H, 5.33; N, 3.23.

Compound 5a: ¹HNMR (CDCl₃, 300MHz): δ 3.51 (s, 3H), 3.79 (s, 3H), 4.38 (s, 1H), 4.90 (s, 1H), 5.37 (d, 1H), 6.13 (d, 1H), 7.04-7.22 (m, 4H), 7.53-7.62 (m, 4H). ¹³C NMR (75 MHz) δ 52.13, 53.21, 66.62, 67.58, 104.32, 122.11, 124.24, 125.31, 126.82, 128.4, 128.9, 129.42, 130.02, 131.12, 132.00, 132.83, 134.35, 137.54, 138.18, 142.53, 167.33, 169.99, 197.47. Anal. Calcd. For C₂₃H₁₈ClNO₅: C, 65.18; H, 4.28; N, 3.30; found C, 65.09; H, 4.22; N, 3.24; m/z: 423.09.

Compound 5b: ¹HNMR (CDCl₃, 300MHz): δ 3.44 (s, 3H), 3.78 (s, 3H), 4.47 (s, 1H), 4.86 (s, 1H), 5.49 (d, 1H), 6.90 (d, 1H), 7.16-7.28 (m, 4H), 7.49-7.62 (m, 4H). ¹³C NMR (75 MHz) δ 52.08, 53.14, 65.84, 67.35, 102.52, 124.32, 125.51, 126.46, 127.57, 128.02, 128.98, 129.80, 130.37, 131.73, 132.65, 133.91, 136.03, 137.14, 137.98, 138.64, 166.31, 169.17, 194.65. Anal. Calcd. For C₂₃H₁₈ClNO₅: C, 65.18; H, 4.28; N, 3.30; found C, 65.12; H, 4.26; N, 3.20; m/z: 423.09.

Compound 5c: ¹HNMR (CDCl₃, 300MHz): δ 3.57 (s, 3H), 3.79 (s, 3H), 3.99 (s, 3H), 4.68 (s, 1H), 4.93 (s, 1H), 5.64 (d, 1H), 6.58 (s, 1H); 6.98-7.20 (m, 4H), 7.68-7.76 (m, 4H). ¹³C NMR (75 MHz) δ 52.36, 53.32, 56.46, 66.48, 68.08, 100.52, 113.67, 118.36, 122.98, 124.73, 125.31, 127.62, 129.00, 130.52, 131.43, 132.84, 133.44, 135.57, 137.36, 138.92, 165.77, 167.47, 171.13, 191.69. Anal. Calcd. For C₂₄H₂₁NO₆: C, 68.73; H, 5.05; N, 3.34; found C, 68.59; H, 5.01; N, 3.24; m/z: 419.14.

Compound 5d: ^1H NMR (CDCl_3 , 300MHz): δ 3.32 (s, 3H), 3.78 (s, 3H), 4.48 (s, 1H), 4.96 (s, 1H), 5.32 (s, 1H), 5.68 (d, 1H), 6.98 (d, 1H), 7.05-7.12 (m, 2H), 7.19-7.48 (m, 6H). ^{13}C NMR (75 MHz) δ 51.98, 53.65, 64.62, 69.25, 106.54, 115.66, 117.37, 121.00, 124.24, 125.75, 126.23, 127.00, 129.08, 130.12, 132.68, 133.73, 134.88, 137.52, 138.26, 164.43, 167.43, 170.11, 200.84. Anal. Calcd. For $\text{C}_{23}\text{H}_{19}\text{NO}_6$: C, 68.14; H, 4.72; N, 3.46; found C, 68.02; H, 4.68; N, 3.30; m/z: 405.12.

Compound 5e: ^1H NMR (CDCl_3 , 300MHz): δ 3.28 (s, 3H), 3.56 (s, 3H), 3.98 (s, 3H), 4.48 (s, 1H), 4.96 (s, 1H), 5.48 (s, 1H), 5.24 (d, 1H), 6.77 (d, 1H), 7.05-7.18 (m, 3H), 7.26-7.38 (m, 4H). ^{13}C NMR (75 MHz) δ 52.01, 53.07, 58.37, 66.58, 70.84, 100.92, 113.46, 115.00, 120.83, 123.86, 124.79, 126.29, 127.08, 129.40, 131.02, 132.92, 133.73, 136.54, 139.62, 142.61, 153.00, 162.41, 171.13, 195.64. Anal. Calcd. For $\text{C}_{24}\text{H}_{21}\text{NO}_7$: C, 66.20; H, 4.86; N, 3.22; found C, 66.14; H, 4.82; N, 3.10; m/z: 435.13.

Compound 5f: ^1H NMR (CDCl_3 , 300MHz): δ 3.51 (s, 3H), 3.79 (s, 3H), 4.58 (s, 1H), 4.96 (s, 1H), 5.48 (d, 1H), 6.92 (d, 1H), 7.18-7.26 (m, 4H), 8.02-8.14 (m, 4H). ^{13}C NMR (75 MHz) δ 54.60, 55.13, 68.36, 69.42, 106.80, 121.36, 122.70, 124.42, 125.31, 126.93, 127.45, 129.12, 130.34, 131.08, 132.00, 135.73, 137.82, 138.46, 145.65, 151.33, 164.43, 171.11, 197.53. Anal. Calcd. For $\text{C}_{23}\text{H}_{18}\text{N}_2\text{O}_7$: C, 63.59; H, 4.18; N, 6.45; found C, 63.53; H, 4.16; N, 6.42; m/z: 434.11.

Compound 5g: ^1H NMR (CDCl_3 , 300MHz): δ 1.53 (t, 3H), 1.72 (t, 3H), 3.92 (q, 2H), 4.17 (q, 2H), 4.68 (s, 1H), 4.98 (s, 1H), 5.42 (d, 1H), 6.86 (d, 1H), 7.17-7.39 (m, 6H), 7.53-7.68 (m, 2H). ^{13}C NMR (75 MHz) δ 15.30, 18.62, 59.37, 62.20, 66.32, 71.68, 98.00, 123.04, 125.63, 126.50, 127.46, 129.00, 129.64, 130.08, 130.78, 131.46, 132.40, 134.75, 135.46, 136.52, 139.21, 142.00, 167.19, 171.18, 193.45. Anal. Calcd. For $\text{C}_{25}\text{H}_{22}\text{ClNO}_5$: C, 66.45; H, 4.91; N, 3.10; found C, 66.31; H, 4.88; N, 3.00; m/z: 451.12.

Compound 5h: ^1H NMR (CDCl_3 , 300MHz): δ 1.38 (t, 3H), 1.84 (t, 3H), 3.25 (s, 3H), 3.98 (q, 2H), 4.23 (q, 2H), 4.56 (s, 1H), 5.00 (s, 1H), 5.41 (d, 1H), 6.84 (d, 1H), 7.04-7.20 (m, 6H), 7.78-7.90 (m, 2H). ^{13}C NMR (75 MHz) δ 14.17, 18.67, 54.36, 61.00, 63.71, 65.60, 69.32, 100.52, 111.69, 114.55, 122.24, 124.63, 126.54, 127.39, 129.39, 130.32, 131.24, 132.57, 133.64, 135.64, 137.00, 141.27, 164.92, 166.73, 170.02, 197.37. Anal. Calcd. For $\text{C}_{26}\text{H}_{25}\text{NO}_6$: C, 69.79; H, 5.63; N, 3.13; found C, 69.71; H, 5.59; N, 3.03; m/z: 447.17.

Compound 5i: ^1H NMR (CDCl_3 , 300MHz): δ 1.40 (t, 3H), 1.97 (t, 3H), 3.71 (q, 2H), 4.05 (q, 2H), 4.68 (s, 1H), 5.02 (s, 1H), 5.73 (d, 1H), 6.81 (d, 1H), 7.15-7.30 (m, 4H), 8.00-8.24 (m, 4H). ^{13}C NMR (75 MHz) δ 16.04, 20.14, 59.44, 62.56, 68.68, 70.24, 102.18, 123.72, 124.96, 125.28, 126.53, 127.09, 128.00, 128.12, 129.38, 130.64, 134.68, 135.88, 137.04, 139.53, 141.65, 151.33, 165.00, 169.82, 195.43. Anal. Calcd. For $\text{C}_{25}\text{H}_{22}\text{N}_2\text{O}_7$: C, 64.93; H, 4.80; N, 6.06; found C, 64.80; H, 4.72; N, 5.92; m/z: 462.14.

Compound 5j: ^1H NMR (CDCl_3 , 300MHz): δ 1.42 (t, 3H), 1.91 (t, 3H), 3.84 (q, 2H), 4.02 (q, 2H), 4.51 (s, 1H), 4.98 (s, 1H), 5.40 (d, 1H), 6.92 (d, 1H), 7.08-7.26 (m, 4H), 7.90-8.16 (m, 4H). ^{13}C NMR (75 MHz) δ 14.20, 19.64, 61.02, 64.00, 69.21, 102.42, 113.64, 119.60, 121.00, 124.32, 125.56, 126.31, 127.82, 129.08, 130.59, 132.40, 134.72, 135.14, 137.55, 139.77, 163.37, 166.09, 169.12, 201.00. Anal. Calcd. For $\text{C}_{25}\text{H}_{23}\text{NO}_6$: Elemental Analysis: C, 69.27; H, 5.35; N, 3.23; found C, 69.20; H, 5.35; N, 3.11; m/z: 433.15.