

1,3-Insertion of amidines into ethyl *E*-2-acyl-3-ferrocenylacrylates

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Ethyl 3-(2-benzoyl-1,1-dimethylguanidino)-3-ferrocenylpropionate 5b. Yield 0.83 g (35%), yellow crystals, mp 202–203 °C. ¹H NMR (CDCl₃, 300 MHz) δ: 1.23 (t, 3H, Me, *J* 7.2 Hz), 2.88 (dd, 1H, CH₂, *J* 4.8 and 16.1 Hz), 2.97 (dd, 1H, CH₂, *J* 5.7 and 16.1 Hz), 3.07 (s, 6H, 2Me), 4.10 (q, 2H, CH₂, *J* 7.2 Hz), 4.14 (s, 5H, C₅H₅), 4.07 (m, 1H, C₅H₄), 4.11 (m, 1H, C₅H₄), 4.17 (m, 1H, C₅H₄), 4.19 (m, 1H, C₅H₄), 5.08 (dd, 1H, CH, *J* 4.8 and 5.7 Hz), 5.47 (br. s, 1H, NH), 7.41 (m, 3H, C₆H₅), 8.23 (d, 2H, Ph, *J* 9.2 Hz). ¹³C NMR (CDCl₃, 75 MHz) δ: 14.20, 36.79 (3Me), 48.59 (CH), 39.92, 61.08 (2CH₂), 68.76 (C₅H₅), 66.17, 67.34, 68.07, 68.31 (C₅H₄), 88.87 (C_{ipso}Fc), 123.04, 129.78 (C₆H₄), 144.38, 149.11, 162.72, 172.21 (4C). MS, *m/z*: 475 [M]⁺. Found (%): C, 63.12; H, 6.23; Fe, 11.68; N, 8.71. Calc. for C₂₅H₂₉FeN₃O₃ (%): C, 63.17; H, 6.15; Fe, 11.75; N, 8.83.

Ethyl 3-[1,1-dimethyl-2-(4-nitrobenzoyl)guanidino]-3-ferrocenylpropionate 5c. Yield 1.09 g (42%), yellow crystals, mp 206–207 °C. ¹H NMR (CDCl₃, 300 MHz) δ: 1.23 (t, 3H, Me, *J* 7.2 Hz), 2.90 (dd, 1H, CH₂, *J* 4.5 and 16.1 Hz), 2.99 (dd, 1H, CH₂, *J* 5.7 and 16.1 Hz), 3.17 (s, 6H, 2Me), 4.13 (q, 2H, CH₂, *J* 7.2 Hz), 4.15 (s, 5H, C₅H₅), 4.09 (m, 1H, C₅H₄), 4.11 (m, 1H, C₅H₄), 4.16 (m, 1H, C₅H₄), 4.18 (m, 1H, C₅H₄), 5.09 (dd, 1H, CH, *J* 4.5 and 5.1 Hz), 5.77 (br. s, 1H, NH), 8.24 (d, 2H, C₆H₄, *J* 9.0 Hz), 8.36 (d, 2H, C₆H₄, *J* 9.0 Hz). ¹³C NMR (CDCl₃, 75 MHz) δ: 14.22, 38.73, (3Me), 49.60 (CH), 40.02, 61.15 (2CH₂), 68.93 (C₅H₅), 66.27, 67.43, 68.15, 68.44 (C₅H₄), 88.95 (C_{ipso}Fc), 123.12, 129.97 (C₆H₄), 144.56, 149.21, 162.88, 167.36, 172.39 (5C). MS, *m/z*: 520 [M]⁺. Found (%): C, 57.49; H, 5.34; Fe, 10.59; N, 10.63. Calc. for C₂₅H₂₈FeN₄O₅ (%): C, 57.71; H, 5.42; Fe, 10.73; N, 10.76.

Ethyl 5-ferrocenyl-3-methyl-7-(4-nitrophenyl)-7-oxo-2,4-diazahept-2-enoate 5e. Yield 0.31 g (13%), orange powder, mp 181–183 °C. ¹H NMR (CDCl₃, 300 MHz) δ: 1.25 (t, 3H, Me, *J* 7.2 Hz), 2.39 (s, 3H, Me), 2.88 (dd, 1H, CH₂, *J* 8.8 and 16.2 Hz), 2.96 (dd, 1H, CH₂, *J* 5.6 and 16.2 Hz), 4.16 (q, 2H, CH₂, *J* 7.2 Hz), 4.20 (s, 5H, C₅H₅), 4.13 (m, 1H, C₅H₄), 4.18 (m, 1H, C₅H₄), 4.22 (m, 1H, C₅H₄), 4.24 (m, 1H, C₅H₄), 5.61 (dd, 1H, CH, *J* 5.6 and 8.8 Hz), 6.44 (br. s, 1H, NH), 8.26 (d, 2H, C₆H₄, *J* 9.3 Hz), 8.35 (d, 2H, C₆H₄, *J* 9.3 Hz). ¹³C NMR (CDCl₃, 75 MHz) δ: 14.26, 21.12 (2Me), 39.52, 61.05 (2CH₂), 47.51 (CH), 68.87 (C₅H₅), 66.52, 67.29, 68.22, 68.52 (C₅H₄), 88.25 (C_{ipso}Fc), 123.23, 130.56 (C₆H₄), 143.13, 149.72, 164.98, 171.45, 174.67 (5C). MS, *m/z*: 491 [M]⁺. Found (%): C, 58.54; H, 5.19; Fe, 11.45; N, 8.37. Calc. for C₂₄H₂₅FeN₃O₅ (%): C, 58.67; H, 5.13; Fe, 11.37; N, 8.55.