Supporting Information

Synthesis of 1,3,5-trisubstituted hydantoins by regiospecific domino condensation/aza-Michael/O → N acyl migration of carbodiimides with activated α,β -unsaturated carboxylic acids

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S-2

S-4

(S,S)-8d ¹H NMR (CDCl₃)

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8g ^1H NMR (CDCl_3)

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S-12

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8n ^1H NMR (CDCl_3)

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Thermal ellipsoid plot (50% probabilità) of 1-benzyl-3-(4-methoxy-phenyl)-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (**12e**).

Crystal data for 12e: C₂₀H₁₆F₆N₂O₃, $M = 446.35$, colourless prism, 0.28 x 0.26 x 0.15 mm, monoclinic, $a = 19.684(4)$, $b = 5.4468(11)$, $c = 20.360(4)$ Å, $\beta = 118.43(3)$, $V = 1919.7(7)$ Å³, $T = 150(2)$ K, space group P2₁/c, $Z = 4$, $\mu(\text{Mo-K}\alpha) = 0.143$ mm⁻¹, Nonius Kappa CCD diffractometer, Mo K α ($\lambda = 0.71073$ Å), 17677 reflections measured, 4737 unique ($R_{\text{int}} = 0.0292$), refinement on F^2 (SHELXL-97, G.M. Sheldrick, University of Göttingen, 1997), 281 parameters, rigid methyl, other hydrogen atoms riding, $R_1[I > 2\sigma(I)] = 0.0353$, $wR_2(\text{all data}) = 0.0902$, max. $\Delta\rho = 0.336$ eÅ⁻³. Full data (excluding structure factors) of the crystal structure have been deposited with Cambridge Crystallographic Data Center as supplementary publication no. 250248. Copies of the data can be obtained, free of charge, on application to CCDC, Union Road, Cambridge, CB2 1EZ, UK [fax: +44(0)-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk]

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Thermal ellipsoid plot (50% probabilità) of (*S,S*)-(2,5-dioxo-1,3-di-*tert*-butyl-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (**8c**).

Crystal data for 8c: C₁₆H₂₅F₃N₂O₄, *M* = 366.38, colourless block, 0.56 x 0.56 x 0.48 mm, monoclinic, *a* = 9.838(2), *b* = 11.258(2), *c* = 17.227(3) Å, β = 106.15(3), *V* = 1832.7(6) Å³, *T* = 150(2) K, space group P2₁/n, *Z* = 4, μ(Mo-Kα) = 0.114 mm⁻¹, Nonius Kappa CCD diffractometer, Mo Kα (λ = 0.71073 Å), 17225 reflections measured, 4521 unique (*R*_{int} = 0.0258), refinement on *F*² (SHELXL-97, G.M. Sheldrick, University of Göttingen, 1997), 233 parameters, rigid methyl, other hydrogen atoms riding, *R*₁[*I* > 2σ(*I*)] = 0.0404, *wR*₂(all data) = 0.1123, max. Δρ = 0.371 eÅ⁻³. Full data (excluding structure factors) of the crystal structure have been deposited with Cambridge Crystallographic Data Center as supplementary publication no. 250249. Copies of the data can be obtained, free of charge, on application to CCDC, Union Road, Cambridge, CB2 1EZ, UK [fax: +44(0)-1223-336033 or e-mail: deposit@ccdc.cam.ac.uk]

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4-(1,3-Di-*tert*-butyl-ureido)-4-oxo-but-2-enoic acid ethyl ester (6k). $R_f = 0.26$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1754, 1733 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 6.54 (d, $J = 11.6$ Hz, 1H), 6.29 (br s, 1H), 5.91 (d, $J = 11.6$ Hz, 1H), 4.22 (q, $J = 7.2$ Hz, 2H), 1.52 (s, 9H), 1.30 (t, $J = 7.2$ Hz, 3H), 1.25 (s, 9H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 166.4, 164.4, 153.1, 139.9, 122.2, 61.2, 57.7, 51.6, 28.0, 27.8, 14.1; EIMS (m/z) 299 [$\text{M}^+ + 1$ (37)], 227 (82), 57 (100).

3-Benzyl-1-(4-methoxy-phenyl)-1-[4-(4-fluoro-phenyl)-4-oxo-but-2-enoyl]-urea (6c). $R_f = 0.49$ (hexane/AcOEt = 60:40); m.p. 144-145 $^\circ\text{C}$; FTIR (microscope) ν 1774, 1723, 1707, 1682 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 9.42 (br s, 1H), 7.92 (m, 2H), 7.81 (d, $J = 15.3$ Hz, 1H), 7.39-7.25 (m, 5H), 6.97 (d, $J = 8.8$ Hz, 2H), 6.78 (d, $J = 15.3$ Hz, 1H), 4.56 (d, $J = 5.7$ Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 187.4, 167.8, 166.1 (d, $J = 255.3$) 160.3, 154.4, 135.0, 133.9, 132.9 (d, $J = 3.7$ Hz), 131.5 (d, $J = 9.2$ Hz), 130.7, 130.4, 129.6, 128.7, 128.1, 127.8, 116.1 (d, $J = 22.2$ Hz), 115.0, 55.5, 44.7; ^{19}F NMR (235.4 MHz, CDCl_3) δ -104.4 (m, 1F); EIMS (m/z) 432 [M^+ (3)], 299 (63), 123 (97), 91 (100).

3-Benzyl-1-(4-methoxy-phenyl)-1-(4-oxo-pent-2-enoyl)-urea (6d). $R_f = 0.39$ (hexane/AcOEt = 70:30); m.p. 105-106 $^\circ\text{C}$; FTIR (microscope) ν 1704, 1645 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 9.33 (br s, 1H), 7.36-7.25 (m, 5H), 7.13 (d, $J = 9.0$ Hz, 2H), 6.97 (m, 3H), 6.55 (d, $J = 15.5$ Hz, 1H), 4.53 (d, $J = 5.7$ Hz, 2H), 3.84 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 196.8, 167.9, 160.1, 154.4, 138.6, 138.0, 132.6, 130.4, 129.7, 128.7, 127.8, 127.5, 115.0, 55.5, 44.7, 28.4; EIMS (m/z) 353 [$\text{M}^+ + 1$ (2)], 352 [M^+ (4)], 219 (100), 91 (96).

3-Cyclohexyl-1-[4-(methoxy-phenyl)-4-oxo-but-2-enoyl]-1-phenyl-urea (6h). $R_f = 0.65$ (hexane/AcOEt = 60:40); FTIR (neat) ν 1738, 1719 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 9.12 (br d, $J = 7.2$ Hz, 1H), 7.88 (m, 3H), 7.43 (m, 3H), 7.22 (m, 2H), 6.91 (d, $J = 8.8$ Hz, 2H), 6.66 (d, $J = 15.0$ Hz, 1H), 3.85 (s, 3H), 3.78 (m, 1H), 2.00 (m, 2H), 1.89 (m, 1H), 1.77-1.54 (m, 4H), 1.42-1.23 (m, 2H), 1.07 (m, 1H); ^{13}C NMR (62.9 MHz, CDCl_3) δ 187.2, 167.8, 164.2, 153.3, 137.4, 135.8,

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133.0, 131.2, 129.6, 129.4, 129.2, 120.0, 114.1, 55.5, 49.5, 33.6, 32.8, 25.6, 24.8, 24.5; EIMS (m/z) 406 [M^+ (9)], 271 (12), 189 (23), 135 (25), 91 (100).

3-Cyclohexyl-1-[4-(fluoro-phenyl)-4-oxo-but-2-enoyl]-1-phenyl-urea (6i). R_f = 0.59 (hexane/AcOEt = 70:30); m.p. 122-123 °C; FTIR (microscope) ν 1729, 1652, 1598 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 9.04 (br d, J = 6.5 Hz, 1H), 7.90 (m, 2H), 7.82 (d, J = 15.0 Hz, 1H), 7.45 (m, 3H), 7.23 (m, 2H), 7.12 (m, 2H), 3.77 (m, 1H), 1.98 (m, 2H), 1.73 (m, 2H), 1.60 (m, 1H), 1.46-1.22 (m, 5H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 187.4, 167.5, 166.1 (d, J = 257.1 Hz), 153.2, 137.2, 135.0, 134.0, 132.9, 131.5 (d, J = 9.2 Hz), 129.7, 129.5, 129.3, 116.0 (d, J = 22.2 Hz), 49.5, 32.8, 32.7, 25.5, 24.6, 24.5; ^{19}F NMR (235.4 MHz, CDCl_3) δ -104.4 (m, 1F); EIMS (m/z) 395 [M^+ +1 (14)], 394 [M^+ (3)], 296 (63), 309 (25), 146 (61), 123 (74), 93 (100).

(S,S)-(1,3-Dicyclohexyl-2,5-dioxo-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (8b). R_f = 0.41 (hexane/AcOEt = 90:10); FTIR (microscope) ν 1764, 1709 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.32-4.18 (m, 2H), 4.30 (d, J = 1.8 Hz, 1H), 3.89 (m, 2H), 3.23 (tt, J = 11.9 and 3.9 Hz, 1H), 2.09 (m, 3H), 1.86-1.60 (m, 11H), 1.37-1.32 (m, 6H), 1.27 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 170.3, 163.1, 156.4, 123.7 (q, J = 279.0 Hz), 62.4, 57.0, 56.4, 52.2, 51.2 (q, J = 27.3 Hz), 30.7, 29.3, 29.1, 28.9, 26.2, 25.9, 25.8, 25.7, 25.1, 25.0, 14.1; ^{19}F NMR (235.4 MHz, CDCl_3) δ -65.3 (d, J = 9.6 Hz, 3F); EIMS (m/z) 419 [M^+ +1 (100)], 375 (26).

(S,R)-(1,3-Dicyclohexyl-2,5-dioxo-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (8b). R_f = 0.29 (hexane/AcOEt = 90:10); FTIR (microscope) ν 1778, 1743, 1714 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.47 (d, J = 1.6 Hz, 1H), 4.30 (m, 2H), 3.88 (m, 2H), 3.21 (tt, J = 11.9 and 3.4 Hz, 1H), 2.08 (m, 3H), 1.81 (m, 6H), 1.63 (m, 5H), 1.32 (t, J = 7.2 Hz, 3H), 1.22 (m, 6H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 170.2, 165.0, 156.4, 123.1 (q, J = 279.2 Hz), 62.9, 56.4, 56.0,

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52.0, 50.4 (q, $J = 27.2$ Hz), 30.2, 29.6, 29.1, 28.8, 26.3, 25.9, 25.8, 25.7, 25.3, 25.0, 14.0; ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.5 (d, $J = 8.3$ Hz, 3F); EIMS (m/z) 419 [$\text{M}^+ + 1$ (68)], 375 (100).

(*S,S*)-(2,5-Dioxo-1,3-di-*tert*-butyl-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (8c). $R_f = 0.51$ (hexane/AcOEt = 80:20); m.p. 84 °C, FTIR (microscope) ν 1751, 1738 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.36 (d, $J = 1.8$ Hz, 1H), 4.32-4.22 (m, 2H), 3.93 (dq, $J = 9.1$ and 1.8 Hz, 1H), 1.58 (s, 9H), 1.40 (s, 9H), 1.31 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 171.0, 165.0, 157.7, 123.1 (q, $J = 280.7$ Hz), 62.6, 58.4, 56.6, 56.3, 52.5 (q, $J = 26.9$ Hz), 28.4, 28.0, 13.9; ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.8 (d, $J = 9.1$ Hz, 3F); EIMS (m/z) 367 [M^+ (45)], 351 (54), 295 (100), 57 (100).

(*S,R*)-(2,5-Dioxo-1,3-di-*tert*-butyl-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (8c). $R_f = 0.42$ (hexane/AcOEt = 80:20); FTIR (microscope) ν 1753, 1712 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.53 (m, 1H), 4.32 (q, $J = 7.0$ Hz, 2H), 3.68 (dq, $J = 8.5$ and 4.1 Hz, 1H), 1.55 (s, 9H), 1.47 (s, 9H), 1.33 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.4, 163.6, 156.9, 123.4 (q, $J = 281.1$ Hz), 62.5, 58.3, 56.7, 56.4, 51.3 (q, $J = 25.9$ Hz), 28.4, 28.2, 13.9; ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.4 (d, $J = 7.6$ Hz, 3F); EIMS (m/z) 368 [$\text{M}^+ + 1$ (9)], 367 [M^+ (37)], 395 (83), 254 (100), 57 (89).

(2,5-Dioxo-1,3-di-*p*-tolyl-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (8d, unseparable mixture): $R_f = 0.59$ (hexane/AcOEt = 70:30); ^1H NMR (400 MHz, CDCl_3) δ 7.35-7.23 (m, 4H), 5.26 (d, $J = 2.3$ Hz, 1H), 4.11 (m, 2H), 3.85 (dq, $J = 9.0$ and 2.3 Hz, 1H), 2.39 (s, 3H), 2.36 (s, 3H), 1.17 (t, $J = 7.2$ Hz, 1H); ^{19}F NMR (235.4 MHz, CDCl_3) δ -64.9 (d, $J = 8.7$ Hz, 3F).

(2,5-Dioxo-1,3-di-*p*-tolyl-imidazolidin-4-yl)-3,3,3-trifluoro-propionic acid ethyl ester (8d, unseparable mixture): $R_f = 0.59$ (hexane/AcOEt = 70:30); ^1H NMR (400 MHz, CDCl_3) δ 7.35-

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7.23 (m, 4H), 5.22 (d, $J = 2.3$ Hz, 1H), 4.33 (m, 2H), 3.98 (dq, $J = 9.0$ and 2.3 Hz, 1H), 2.39 (s, 3H), 2.36 (s, 3H), 1.31 (t, $J = 7.2$ Hz, 3H); ^{19}F NMR (235.4 MHz, CDCl_3) δ -67.2 (d, $J = 8.7$ Hz, 3F).

2-(1,3-Diisopropyl-2,5-dioxo-imidazolidin-4-yl)-malonic acid diethyl ester (8e). $R_f = 0.35$ (hexane/AcOEt = 70:30); m.p. 60-62 °C; FTIR (microscope) ν 1769, 1750, 1733, 1725 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.42 (d, $J = 3.6$ Hz, 1H), 4.27 (m, 3H), 4.03 (septet, $J = 6.7$ Hz, 1H), 4.00 (d, $J = 3.6$ Hz, 1H), 1.42 (d, $J = 7.0$ Hz, 3H), 1.34 (d, $J = 7.0$ Hz, 3H), 1.30 (t, $J = 7.0$ Hz, 3H), 1.28 (t, $J = 7.0$ Hz, 3H), 1.26 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 170.5, 166.0, 165.7, 156.4, 62.3, 61.9, 56.8, 52.9, 45.8, 44.0, 20.7, 19.9, 19.5, 19.3, 14.0, 13.9; EIMS (m/z) 342 [M^+ (17)], 269 (20), 223 (100).

2-(1,3-Dicyclohexyl-2,5-dioxo-imidazolidin-4-yl)-malonic acid diethyl ester (8f). $R_f = 0.51$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1772, 1746, 1718 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.43 (d, $J = 3.9$ Hz, 1H), 4.25 (m, 2H), 3.98 (d, $J = 3.9$ Hz, 1H), 3.89 (tt, $J = 12.4$ and 3.9 Hz, 1H), 3.62 (m, 1H), 2.12 (m, 2H), 1.88-1.59 (m, 11H), 1.51 (m, 1H), 1.36-1.11 (m, 6H), 1.31 (t, $J = 7.2$ Hz, 3H), 1.27 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 170.7, 165.9, 165.7, 156.6, 62.3, 61.8, 56.8, 53.9, 53.0, 51.9, 31.3, 30.4, 29.2, 29.0, 26.0, 25.9, 25.8, 25.3, 25.1, 14.1, 14.0; EIMS (m/z) 423 [$\text{M}^+ + 1$ (100)], 349 (75), 303 (98).

2-(1,3-Di-*tert*-butyl-2,5-dioxo-imidazolidin-4-yl)-malonic acid diethyl ester (8g). $R_f = 0.57$ (hexane/AcOEt = 70:30); m.p. 88-90 °C; FTIR (microscope) ν 1774, 1768, 1747, 1697 cm^{-1} ; ^1H NMR (400 MHz, CD_2Cl_2) δ 4.39 (d, $J = 4.4$ Hz, 1H), 4.23 (m, 2H), 4.00 (d, $J = 4.4$ Hz, 1H), 1.56 (s, 9H), 1.41 (s, 9H), 1.29 (t, $J = 7.0$ Hz, 3H), 1.26 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CD_2Cl_2) δ 172.8, 168.0, 167.8, 159.7, 63.9, 63.5, 59.3, 57.7, 56.8, 30.2, 30.1, 15.9, 15.7; EIMS (m/z) 342 [M^+ (17)], 269 (20), 223 (100).

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(1,3-Diisopropyl-2,5-dioxo-imidazolidin-4-yl)-acetic acid ethyl ester (8i). $R_f = 0.38$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1766, 1732, 1694 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.28 (septet, $J = 7.0$ Hz, 1H), 4.12 (m, 3H), 4.01 (dd, $J = 5.1$ and 3.5 Hz, 1H), 2.96 (dd, $J = 16.8$ and 3.5 Hz, 1H), 2.82 (dd, $J = 16.8$ and 5.1 Hz, 1H), 1.40 (d, $J = 3.1$ Hz, 3H), 1.38 (d, $J = 3.1$ Hz, 3H), 1.25 (d, $J = 6.6$ Hz, 3H), 1.21 (t, $J = 7.0$ Hz, 3H), 1.20 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (62.9 MHz, CDCl_3) δ 172.2, 168.8, 156.2, 61.0, 54.2, 44.8, 43.9, 35.4, 21.4, 19.7, 19.6, 19.2, 14.1; EIMS (m/z) 271 [$\text{M}^+ + 1$, 20], 270 [M^+ , 100], 196 (58), 70 (65).

(1,3-Dicyclohexyl-2,5-dioxo-imidazolidin-4-yl)-acetic acid ethyl ester (8j). $R_f = 0.49$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1772, 1729, 1693 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.14 (m, 2H), 4.04 (dd, $J = 5.4$ and 3.6 Hz, 1H), 3.89 (tt, $J = 12.4$ and 3.9 Hz, 1H), 3.67 (tt, $J = 12.2$ and 3.9 Hz, 1H), 2.96 (dd, $J = 16.8$ and 3.6 Hz, 1H), 2.83 (dd, $J = 6.8$ and 5.4 Hz, 1H), 2.12 (m, 2H), 1.85-1.60 (m, 11H), 1.50-1.10 (m, 7H), 1.22 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 172.4, 168.9, 156.4, 61.0, 54.6, 53.2, 51.8, 35.8, 31.9, 30.4, 29.3, 29.1, 25.92, 25.90, 25.3, 25.2, 14.2; EIMS (m/z) 337 [$\text{M}^+ + 1$, 34], 236 [M^+ , 100].

(1,3-Di-*tert*-butyl-2,5-dioxo-imidazolidin-4-yl)-acetic acid ethyl ester (8k). $R_f = 0.48$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1761, 1737, 1704 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.15 (m, 2H), 3.98 (dd, $J = 6.5$ and 2.3 Hz, 1H), 3.05 (dd, $J = 16.0$ and 2.3 Hz, 1H), 2.81 (dd, $J = 16.0$ and 6.5 Hz, 1H), 1.60 (s, 9H), 1.42 (s, 9H), 1.25 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 173.0, 168.9, 157.5, 60.9, 57.9, 55.5, 55.4, 38.2, 29.5, 28.7, 28.4, 14.3; EIMS (m/z) 298 [M^+ (100)], 227 (54).

(2,5-dioxo-1,3-di-*p*-tolyl-imidazolidin-4-yl)-acetic acid ethyl ester (8l). $R_f = 0.48$ (hexane/AcOEt = 70:30); m.p. 130-131 $^\circ\text{C}$; FTIR (microscope) ν 1774, 1742, 1692 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.38 (d, $J = 8.3$ Hz, 2H), 7.28 (m, 4H), 7.21 (d, $J = 8.3$ Hz, 2H), 4.82 (dd, $J =$

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4.6 and 3.6 Hz, 1H), 4.09 (m, 2H), 3.05 (dd, $J = 17.1$ and 3.6 Hz, 1H), 2.89 (dd, $J = 17.1$ and 4.6 Hz, 1H), 2.39 (s, 3H), 2.35 (s, 3H), 1.17 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 170.6, 168.6, 154.0, 138.3, 136.1, 132.5, 130.0, 129.7, 129.2, 126.2, 123.2, 61.2, 57.0, 33.4, 21.1, 20.9, 14.0; EIMS (m/z) 366 [M^+ (89)], 292 (82), 91 (100).

1,3-Dicyclohexyl-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (8m). $R_f = 0.57$ (hexane/AcOEt = 60:40); FTIR (neat) ν 1757, 1699, 1600 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.87 (d, $J = 8.8$ Hz, 2H), 6.91 (d, $J = 8.8$ Hz, 2H), 4.32 (dd, $J = 4.4$ and 4.1 Hz, 1H), 3.91 (tq, $J = 12.2$ and 3.6 Hz, 1H), 3.84 (s, 3H), 3.62 (m, 1H), 3.59 (dd, $J = 17.8$ and 4.1 Hz, 1H), 3.35 (dd, $J = 17.8$ and 4.4 Hz, 1H), 2.13 (m, 2H), 1.84-1.55 (m, 11H), 1.38-1.14 (m, 6H), 1.04 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.6, 173.3, 163.9, 156.5, 130.3, 129.4, 113.9, 55.4, 54.1, 53.3, 51.7, 39.1, 31.5, 30.3, 29.3, 29.1, 25.9, 25.8, 25.2, 25.1; EIMS (m/z) 412 [M^+ (30)], 277 (61), 195 (58), 135 (100).

1,3-Diisopropyl-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (8n). $R_f = 0.34$ (hexane/AcOEt = 60:40); m.p. 103-104 $^\circ\text{C}$; FTIR (microscope) ν 1755, 1704, 1689, 1674, 1599 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, $J = 8.8$ Hz, 2H), 6.91 (d, $J = 8.8$ Hz, 2H), 4.32 (m, 2H), 4.07 (septet, $J = 7.0$ Hz, 1H), 3.84 (s, 3H), 3.60 (dd, $J = 18.0$ and 3.7 Hz, 1H), 3.38 (dd, $J = 18.0$ and 4.8 Hz, 1H), 1.45 (d, $J = 6.6$ Hz, 3H), 1.43 (d, $J = 6.6$ Hz, 3H), 1.25 (d, $J = 7.0$ Hz, 3H), 1.12 (d, $J = 7.0$ Hz, 3H), 1.10 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.5, 173.2, 163.9, 156.3, 130.3, 129.2, 113.9, 55.5, 53.9, 44.9, 43.9, 39.0, 23.4, 21.1, 19.8, 19.5, 19.4; EIMS (m/z) 332 [M^+ (36)], 197 (55), 155 (60), 135 (100).

5-[2-(4-Methoxy-phenyl)-2-oxo-ethyl]-1,3-di-*p*-tolyl-imidazolidine-2,4-dione (8o). $R_f = 0.35$ (hexane/AcOEt = 60:40); m.p. 155-156 $^\circ\text{C}$; FTIR (microscope) ν 1778, 1732, 1683, 1673, 1602 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.77 (d, $J = 8.8$ Hz, 2H), 7.46 (d, $J = 8.3$ Hz, 2H), 7.30

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(d, $J = 8.3$ Hz, 2H), 7.14 (d, $J = 8.3$ Hz, 2H), 6.85 (d, $J = 8.8$ Hz, 2H), 5.01 (dd, $J = 4.4$ and 3.6 Hz, 1H), 3.82 (s, 3H), 3.63 (dd, $J = 18.1$ and 3.6 Hz, 1H), 3.51 (dd, $J = 18.1$ and 3.6 Hz, 1H), 2.39 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.4, 171.6, 163.9, 154.3, 138.2, 135.8, 132.7, 130.3, 129.9, 129.7, 129.5, 129.1, 126.5, 123.2, 113.8, 56.7, 55.5, 36.5, 21.2, 20.9; EIMS (m/z) 428 [M^+ (14)], 293 (100), 135 (58), 91 (62).

1,3-Dicyclohexyl-5-[2-(4-fluoro-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (8p). $R_f = 0.55$ (hexane/AcOEt = 60:40); FTIR (neat) ν 1759, 1694, 1599 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.94 (m, 2H), 7.13 (m, 2H), 4.33 (dd, $J = 4.4$ Hz both, 1H), 3.92 (tq, $J = 12.1$ and 3.9 Hz, 1H), 3.65 (m, 1H), 3.61 (dd, $J = 18.1$ and 4.4 Hz, 1H), 3.40 (dd, $J = 18.1$ and 4.4 Hz, 1H), 2.14 (m, 2H), 1.85-1.60 (m, 12H), 1.27 (m, 5H), 1.06 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.6, 173.2, 166.1 (d, $J = 255.2$ Hz), 156.5, 132.8 (d, $J = 3.1$ Hz), 130.7 (d, $J = 9.4$ Hz), 116.0 (d, $J = 21.8$ Hz), 54.0, 53.3, 51.8, 39.4, 31.7, 30.4, 29.3, 29.1, 25.9, 25.89, 25.86, 25.3, 25.2; ^{19}F NMR (235.4 MHz, CDCl_3) δ -105.1 (quintet, $J = 6.1$ Hz, 1F); EIMS (m/z) 401 [$\text{M}^+ + 1$ (19)], 400 [M^+ (37)], 195 (50), 123 (58), 55 (100).

1,3-Diisopropyl-5-[2-(4-fluoro-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (8q). $R_f = 0.48$ (hexane/AcOEt = 60:40); m.p. 120-130 $^\circ\text{C}$; FTIR (microscope) ν 1755, 1711, 1685, 1597 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.95 (m, 2H), 7.14 (m, 2H), 4.35 (septet, $J = 7.0$ Hz, 1H), 4.32 (dd, $J = 4.8$ and 4.0 Hz, 1H), 4.10 (septet, $J = 6.6$ Hz, 1H), 3.63 (dd, $J = 17.8$ and 4.0 Hz, 1H), 3.42 (dd, $J = 17.8$ and 4.8 Hz, 1H), 1.47 (d, $J = 6.6$ Hz, 3H), 1.45 (d, $J = 6.6$ Hz, 3H), 1.27 (d, $J = 7.0$ Hz, 3H), 1.14 (d, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.6, 173.0, 166.1 (d, $J = 255.7$ Hz), 156.3, 132.7 (d, $J = 3.1$ Hz), 130.7 (d, $J = 9.5$ Hz), 116.0 (d, $J = 22.0$ Hz), 53.8, 45.0, 44.0, 39.3, 21.2, 19.9, 19.6, 19.4; EIMS (m/z) 321 [$\text{M}^+ + 1$ (48)], 320 [M^+ (87)], 197 (84), 123 (100), 95 (79).

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1,3-Dicyclohexyl-5-(2-oxo-propyl)-imidazolidine-2,4-dione (8r). $R_f = 0.54$ (hexane/AcOEt = 60:40); m.p. 80-82 °C; FTIR (microscope) ν 1760, 1717 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.07 (dd, $J = 4.6$ and 4.1 Hz, 1H), 3.85 (tq, $J = 12.2$ and 3.9 Hz, 1H), 3.60 (m, 1H), 3.01 (dd, $J = 18.1$ and 4.6 Hz, 1H), 2.90 (dd, $J = 18.1$ and 4.1 Hz, 1H), 2.15 (s, 3H), 2.08 (m, 2H), 1.82-1.56 (m, 12H), 1.40-1.13 (m, 6H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 203.3, 172.9, 156.3, 53.8, 53.2, 51.7, 43.9, 31.7, 30.3, 30.2, 29.2, 29.0, 25.8, 25.7, 25.2, 25.1; EIMS (m/z) 320 [M^+ (100)], 277 (62), 195 (60), 55 (79).

5-(2-Oxo-propyl)-1,3-di-*p*-tolyl-imidazolidine-2,4-dione (8s). $R_f = 0.11$ (hexane/AcOEt = 80:20); FTIR (neat) ν 1777, 1716 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.39 (d, $J = 8.3$ Hz, 2H), 7.26 (m, 4H), 7.20 (d, $J = 8.5$ Hz, 2H), 4.81 (dd, $J = 4.1$ Hz both, 1H), 3.06 (d, $J = 4.1$ Hz, 2H), 2.38 (s, 3H), 2.35 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 203.5, 171.2, 154.1, 138.3, 136.0, 132.6, 130.0, 129.7, 129.3, 126.4, 123.0, 56.4, 41.2, 30.0, 21.2, 21.0; EIMS (m/z) 336 [M^+ (58)], 293 (100), 132 (59), 91 (57).

1,3-Dicyclohexyl-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (8t). $R_f = 0.73$ (hexane/AcOEt = 80:20); FTIR (neat) ν 1770, 1714 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 4.22 (s, 1H), 3.86 (tq, $J = 12.2$ and 3.6 Hz, 1H), 3.77 (septet, $J = 9.1$ Hz, 1H), 3.11 (tq, $J = 11.9$ and 3.9 Hz, 1H), 2.20 (m, 2H), 2.05 (m, 2H), 1.92-1.58 (m, 11H), 1.22 (m, 6H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.1, 156.3, 122.9 (q, $J = 279.2$ Hz), 122.1 (q, $J = 280.9$ Hz), 57.4, 55.5, 52.4, 49.8 (septet, $J = 27.7$ Hz), 30.4, 29.1, 28.7, 28.5, 26.4, 25.9, 25.8, 25.7, 25.2, 25.0; ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.9 (quintet, $J = 9.1$ Hz, 3F), -64.2 (quintet, $J = 9.1$ Hz, 3F); EIMS (m/z) 414 [M^+ (16)], 333 (100), 251 (67), 55 (82).

1,3-Di-*p*-tolyl-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (8u). $R_f = 0.29$ (hexane/AcOEt = 90:10); m.p. 107-108 °C; FTIR (microscope) ν 1789, 1731 cm^{-1} ; ^1H NMR

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(250 MHz, CDCl_3) δ 7.25 (m, 8H), 5.15 (s, 1H), 3.81 (septet, $J = 8.8$ Hz, 1H), 2.37 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 167.2, 154.0, 139.0, 137.7, 131.9, 130.0, 129.9, 128.5, 125.9, 124.7, 122.4 (q, $J = 280.9$ Hz), 56.2, 49.0 (quintet, $J = 28.8$ Hz), 21.1, 21.0; ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.8 (quintet, $J = 9.5$ Hz, 3F), -64.3 (quintet, $J = 7.6$ Hz, 3F); EIMS (m/z) 430 [M^+ (58)], 118 (87), 91 (100).

[3-Benzyl-1-(4-methoxy-phenyl)-2,5-dioxo-imidazolidin-4-yl]-acetic acid ethyl ester (12a). $R_f = 0.64$ (hexane:AcOEt = 50:50); FTIR (neat) ν 1771, 1737, 1730, 1713 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.84 (d, $J = 9.0$ Hz, 2H), 7.35-7.20 (m, 5H), 6.91 (d, $J = 9.0$ Hz, 2H), 4.78 (d, $J = 14.5$ Hz, 1H), 4.74 (d, $J = 14.5$ Hz, 1H), 4.68 (dd, $J = 5.2$ and 4.1 Hz, 1H), 4.04-3.89 (m, 2H), 3.80 (s, 3H), 2.90 (dd, $J = 16.8$ and 4.1 Hz, 1H), 2.78 (dd, $J = 16.8$ and 5.2 Hz, 1H), 1.10 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 171.2, 168.6, 158.0, 154.8, 135.9, 129.0, 128.6, 127.9, 125.2, 114.6, 61.2, 57.5, 55.5, 42.9, 33.5, 14.0; EIMS (m/z) 382 [M^+ (23)], 91 (100).

1-Benzyl-3-(4-methoxy-phenyl)-5-[2-(4-fluoro-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (12c). $R_f = 0.29$ (hexane/AcOEt = 60:40); m.p. 111-113 $^\circ\text{C}$; FTIR (microscope) ν 1776, 1725, 1681 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.74 (m, 2H), 7.44 (d, $J = 9.0$ Hz, 2H), 7.29-6.99 (m, 9H), 4.63 (d, $J = 15.2$ Hz, 1H), 4.57 (d, $J = 15.2$ Hz, 1H), 4.47 (dd, $J = 5.2$ and 3.4 Hz, 1H), 3.83 (s, 3H), 3.50 (dd, $J = 18.1$ and 3.4 Hz, 1H), 3.34 (dd, $J = 18.1$ and 5.2 Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.4, 172.2, 165.9 (d, $J = 255.2$ Hz), 159.2, 156.5, 136.0, 132.0 (d, $J = 3.7$ Hz), 130.6 (d, $J = 9.2$ Hz), 128.7, 128.0, 127.8, 127.7, 115.6 (d, $J = 22.2$ Hz), 114.4, 55.8, 55.4, 45.8, 38.0; EIMS (m/z) 432 [M^+ (22)], 309 (25), 123 (57), 91 (100).

1-Benzyl-3-(4-methoxy-phenyl)-5-(2-oxo-propyl)-imidazolidine-2,4-dione (12d). $R_f = 0.28$ (hexane/AcOEt = 70:30); FTIR (microscope) ν 1773, 1714, 1516 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.28 (m, 7H), 7.00 (d, $J = 9.0$ Hz, 2H), 4.73 (d, $J = 15.5$ Hz, 1H), 4.46 (d, $J = 15.5$

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Hz, 1H), 4.29 (dd, $J = 5.4$ and 3.4 Hz, 1H), 3.83 (s, 3H), 2.96 (dd, $J = 18.4$ and 3.4 Hz, 1H), 2.85 (dd, $J = 18.4$ and 3.4 Hz, 1H), 1.81 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 203.6, 172.0, 159.3, 156.4, 136.6, 128.9, 128.2, 128.0, 127.7, 124.7, 114.4, 55.9, 55.5, 46.1, 42.7, 29.4; EIMS (m/z) 353 [$\text{M}^+ + 1$ (4)], 352 [M^+ (43)], 91 (100).

1-Benzyl-3-(4-methoxy-phenyl)-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (12e). $R_f = 0.62$ (hexane/AcOEt = 70:30); m.p. 105°C ($i\text{Pr}_2\text{O}$); FTIR (microscope) ν 1791, 1743, 1701 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.34 (m, 3H), 7.30-7.24 (m, 3H), 6.99 (d, $J = 9.0$ Hz, 2H), 5.45 (d, $J = 15.5$ Hz, 1H), 4.31 (s, 3H), 4.10 (d, $J = 15.5$ Hz, 1H), 3.91 (septet, $J = 8.5$ Hz, 1H), 3.84 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 168.8, 159.9, 156.6, 134.6, 129.3, 128.7, 128.4, 127.4, 123.9, 122.8 (q, $J = 281.9$ Hz), 122.3 (q, $J = 285.9$ Hz), 114.7, 55.6, 53.8, 49.8 (septet, $J = 27.6$ Hz), 46.1; ^{19}F NMR (235.4 MHz, CDCl_3) δ -64.4 (quintet, $J = 8.7$ Hz, 3F), -64.8 (quintet, $J = 8.7$ Hz, 3F); EIMS (m/z) 446 [M^+ (44)], 91 (100).

2-(3-Cyclohexyl-2,5-dioxo-1-phenyl-imidazolidin-4-yl)-malonic acid diethyl ester (12f). $R_f = 0.34$ (hexane/AcOEt = 80:20); FTIR (neat) ν 1776, 1737, 1713, 1599 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.43-7.32 (m, 4H), 7.24 (m, 1H), 5.01 (d, $J = 4.4$ Hz, 1H), 4.28 (m, 2H), 4.05 (m, 3H), 3.91 (d, $J = 4.4$ Hz, 1H), 2.20 (m, 2H), 1.83 (m, 4H), 1.66 (m, 1H), 1.30 (t, $J = 7.2$ Hz, 3H), 1.29 (m, 3H), 1.15 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.7, 164.7, 165.5, 154.9, 135.0, 129.4, 126.3, 123.4, 62.4, 61.8, 58.2, 52.3, 50.9, 29.1, 29.0, 25.9, 25.8, 25.1, 14.0, 13.9; EIMS (m/z) 416 [M^+ (50)], 343 (43), 297 (48), 104 (57), 83 (100).

(3-Cyclohexyl-2,5-dioxo-1-phenyl-imidazolidin-4-yl)-acetic acid ethyl ester (12g). $R_f = 0.62$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1770, 1734, 1713, 1599 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.37 (m, 4H), 7.20 (m, 1H), 4.66 (dd, $J = 5.2$ and 3.9 Hz, 1H), 4.03 (m, 3H), 2.93 (dd, $J = 16.8$ and 3.9 Hz, 1H), 2.80 (dd, $J = 16.8$ and 4.2 Hz, 1H), 2.20 (m, 2H), 1.82 (m, 4H), 1.67 (m, 1H),

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1.30 (m, 3H), 1.14 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 171.2, 168.6, 154.7, 135.4, 129.3, 125.8, 122.7, 61.1, 56.1, 52.2, 33.4, 29.2, 29.1, 25.92, 25.90, 25.1, 14.0; EIMS (m/z) 344 [M^+ (100)], 104 (82), 55 (95).

1-Cyclohexyl-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-3-phenyl-imidazolidine-2,4-dione

(12h). $R_f = 0.45$ (hexane/AcOEt = 50:50); FTIR (neat) ν 1767, 1719, 1676, 1602 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.92 (d, $J = 8.8$ Hz, 2H), 7.52 (m, 2H), 7.45 (m, 2H), 7.34 (m, 1H), 6.95 (d, $J = 8.8$ Hz, 2H), 4.54 (dd, $J = 4.4$ and 4.1 Hz, 1H), 3.87 (s, 3H), 3.76 (dd, $J = 18.1$ and 4.1 Hz, 1H), 3.74 (m, 1H), 3.52 (dd, $J = 18.1$ and 4.4 Hz, 1H), 1.86-1.59 (m, 6H), 1.44 (dq, $J = 12.1$ and 3.4 Hz, 1H), 1.27 (m, 2H), 1.10 (m, 1H); ^{13}C NMR (62.9 MHz, CDCl_3) δ 193.4, 172.6, 164.0, 155.5, 132.3, 130.4, 129.1, 128.9, 127.9, 126.4, 114.0, 55.5, 54.6, 53.4, 38.9, 31.6, 30.3, 25.8, 25.2; EIMS (m/z) 406 [M^+ (38)], 271 (69), 189 (94), 135 (61), 55 (100).

1-Cyclohexyl-5-[2-(4-fluoro-phenyl)-2-oxo-ethyl]-3-phenyl-imidazolidine-2,4-dione (12i).

$R_f = 0.26$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1770, 1715, 1599 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.97 (m, 2H), 7.48 (m, 4H), 7.36 (m, 1H), 7.16 (m, 2H), 4.53 (dd, $J = 4.1$ Hz both, 1H), 3.77 (dd, $J = 18.1$ and 4.1 Hz, 1H), 3.76 (m, 1H), 3.56 (dd, $J = 18.1$ and 4.1 Hz, 1H), 1.86-1.60 (m, 6H), 1.46-1.23 (m, 3H), 1.03 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.5, 172.3, 166.1 (d, $J = 257.1$), 155.4, 132.5 (d, $J = 3.7$ Hz), 132.2, 130.7 (d, $J = 9.2$ Hz), 129.0, 128.0, 126.4, 116.0 (d, $J = 22.2$ Hz), 54.4, 53.4, 39.1, 31.7, 30.4, 25.8, 25.2; ^{19}F NMR (235.3 MHz, CDCl_3) δ -104.9 (m, 1F); EIMS (m/z) 395 [$\text{M}^+ + 1$ (37)], 394 [M^+ (80)], 271 (100).

1-Cyclohexyl-3-phenyl-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-

dione (12j). $R_f = 0.75$ (hexane/AcOEt = 80:20); m.p. 129-131 $^\circ\text{C}$; FTIR (microscope) ν 1778, 1716 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.49-7.32 (m, 5H), 4.51 (s, 1H), 3.90 (septet, $J = 8.2$ Hz, 1H), 3.24 (tq, $J = 11.6$ and 3.9 Hz, 1H), 2.30 (m, 1H), 2.01-1.79 (m, 5H), 1.67 (m, 1H), 1.25 (m, 3H); ^{13}C

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NMR (100.6 MHz, CDCl₃) δ 168.3, 155.0, 131.0, 129.2, 128.7, 126.0, 122.8 (q, J = 282.9 Hz), 122.1 (q, J = 284.8 Hz), 57.7, 56.0, 49.9 (septet, J = 27.7 Hz), 30.1, 28.6, 26.3, 25.9, 25.1; ¹⁹F NMR (235.4 MHz, CDCl₃) δ -63.9 (m, 3F), -64.2 (m, 3F); EIMS (m/z) 408 [M^+ (19)], 327 (100).

2-(3-Benzyl-1-*tert*-butyl-2,5-dioxo-imidazolidin-4-yl)-malonic acid diethyl ester (12k). R_f = 0.65 (hexane/AcOEt = 70:30); m.p. 94-96 °C; FTIR (microscope) ν 1770, 1739, 1701 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.35-7.25 (m, 5H), 4.76 (d, J = 15.6 Hz, 1H), 4.32 (d, J = 15.6 Hz, 1H), 4.26 (d, J = 3.2 Hz, 1H), 4.20 (m, 3H), 4.09 (m, 1H), 3.86 (d, J = 3.2 Hz, 1H), 1.63 (s, 9H), 1.25 (t, J = 7.3 Hz, 3H), 1.21 (t, J = 7.1 Hz, 3H); ¹³C NMR (100.6 MHz, CDCl₃) δ 171.3, 166.4, 165.8, 157.9, 136.3, 128.8, 128.2, 62.4, 61.9, 58.3, 57.4, 52.4, 45.4, 28.6, 14.0, 13.98, 13.93; EIMS (m/z) 404 [M^+ (28)], 348 (27), 275 (32), 229 (33), 91 (100).

(3-Benzyl-1-*tert*-butyl-2,5-dioxo-imidazolidin-4-yl)-acetic acid ethyl ester (12l). R_f = 0.58 (hexane/AcOEt = 70:30); FTIR (neat) ν 1767, 1730, 1713 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.35-7.21 (m, 5H), 4.74 (d, J = 15.2 Hz, 1H), 4.27 (d, J = 15.2 Hz, 1H), 4.05 (m, 2H), 3.88 (dd, J = 4.6 and 4.4 Hz, 1H), 2.74 (dd, J = 16.8 and 4.6 Hz, 1H), 2.68 (dd, J = 16.8 and 4.4 Hz, 1H), 1.64 (s, 9H), 1.18 (t, J = 7.0 Hz, 3H); ¹³C NMR (100.6 MHz, CDCl₃) δ 172.8, 169.1, 157.6, 136.3, 128.8, 128.0, 127.9, 61.0, 58.0, 55.4, 45.2, 34.4, 28.7, 14.1; EIMS (m/z) 332 [M^+ (21)], 276 (43), 106 (42), 91 (100).

1-Benzyl-3-*tert*-butyl-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (12m). R_f = 0.58 (hexane/AcOEt = 60:40); FTIR (neat) ν 1765, 1710, 1699, 1600 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.74 (d, J = 8.8 Hz, 2H), 7.21-7.10 (m, 5H), 6.86 (d, J = 8.8 Hz, 2H), 4.60 (d, J = 14.7 Hz, 1H), 4.34 (d, J = 14.7 Hz, 1H), 4.20 (dd, J = 5.9 and 3.6 Hz, 1H), 3.84 (s, 3H), 3.35 (dd, J = 17.8 and 3.6 Hz, 1H), 3.17 (dd, J = 17.8 and 5.9 Hz, 1H), 1.67 (s, 9H); ¹³C NMR (100.6

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MHz, CDCl₃) δ 193.8, 173.8, 163.8, 157.8, 136.6, 130.3, 129.2, 128.6, 128.1, 127.6, 133.7, 55.5, 55.3, 45.4, 38.4, 28.7; EIMS (m/z) 394 [M^+ (22)], 338 (27), 203 (38), 135 (62), 91 (100).

1-Benzyl-3-*tert*-butyl-5-[2-(4-fluoro-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (12n).

R_f = 0.55 (hexane/AcOEt = 60:40); FTIR (neat) ν 1766, 1708, 1699, 1599 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.74 (m, 2H), 7.20-7.03 (m, 7H), 4.51 (d, J = 15.2 Hz, 1H), 4.45 (d, J = 15.2 Hz, 1H), 4.21 (dd, J = 5.9 and 3.6 Hz, 1H), 3.34 (dd, J = 17.8 and 3.6 Hz, 1H), 3.17 (dd, J = 17.8 and 5.9 Hz, 1H), 1.67 (s, 9H); ¹³C NMR (62.9 MHz, CDCl₃) δ 193.8, 173.6, 165.9 (d, J = 255.2 Hz), 157.8, 136.5, 132.3 (d, J = 2.9 Hz), 130.6 (d, J = 11.1 Hz), 128.6, 127.9, 127.6, 115.6 (d, J = 22.2 Hz), 57.9, 55.3, 45.5, 38.5, 28.6; ¹⁹F NMR (235.4 MHz, CDCl₃) δ -105.4 (m, 1F); EIMS (m/z) 382 [M^+ (18)], 326 (27), 203 (60), 123 (74), 91 (100).

1-Benzyl-3-*tert*-butyl-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione

(12o). R_f = 0.78 (hexane/AcOEt = 80:20); m.p. 58-60 °C; FTIR (microscope) ν 1778, 1713 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 7.34 (m, 3H), 7.18 (m, 2H), 5.36 (d, J = 15.5 Hz, 1H), 4.00 (s, 1H), 3.96 (d, J = 15.5 Hz, 1H), 3.80 (septet, J = 9.3 Hz, 1H), 1.62 (s, 9H); ¹³C NMR (100.6 MHz, CDCl₃) δ 170.1, 158.0, 134.8, 129.1, 128.3, 128.1, 122.9 (q, J = 277.4 Hz), 122.3 (q, J = 284.8 Hz), 59.2, 53.3, 49.6 (septet, J = 27.7 Hz), 45.5, 28.3; ¹⁹F NMR (235.4 MHz, CDCl₃) δ -64.6 (m, 3F), -65.2 (m, 3F); EIMS (m/z) 396 [M^+ (28)], 340 (37), 106 (70), 91 (100).

2-[3-(4-Methoxy-phenyl)-1-(4-nitro-phenyl)-2,5-dioxo-imidazolidin-4-yl]-malonic acid diethyl ester (12p). R_f = 0.35 (hexane/AcOEt = 70:30); m.p. 177-178 °C (*i*Pr₂O/AcOEt); FTIR (microscope) ν 1726, 1516 cm⁻¹; ¹H NMR (400 MHz, CDCl₃) δ 8.31 (d, J = 9.1 Hz, 2H), 7.68 (d, J = 9.1 Hz, 2H), 7.39 (d, J = 8.8 Hz, 2H), 7.00 (d, J = 8.8 Hz, 2H), 5.33 (d, J = 4.0 Hz, 1H), 4.32 (m, 2H), 4.18 (m, 1H), 4.09 (m, 1H), 4.08 (d, J = 4.0 Hz, 1H), 3.83 (s, 3H), 1.32 (t, J = 7.1 Hz, 3H), 1.18 (t, J = 7.1 Hz, 3H); ¹³C NMR (100.6 MHz, CDCl₃) δ 168.1, 165.4, 165.1, 159.9, 153.9, 144.8,

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140.8, 127.9, 125.2, 123.7, 121.5, 114.6, 63.0, 62.4, 57.9, 55.6, 50.9, 14.0, 13.9; EIMS (m/z) 486 [$M^+ + 1$, (43)], 485 [M^+ , (81)], 366 (100).

[3-(4-Methoxy-phenyl)-1-(4-nitro-phenyl)-2,5-dioxo-imidazolidin-4-yl]-acetic acid ethyl ester (12q). R_f = 0.19 (hexane/AcOEt = 70:30); ^1H NMR (400 MHz, CDCl_3) δ 8.33 (d, J = 9.0 Hz, 2H), 7.81 (d, J = 9.0 Hz, 2H), 7.26 (d, J = 9.0 Hz, 2H), 6.96 (d, J = 9.0 Hz, 2H), 4.77 (dd, J = 4.4 and 2.6 Hz, 1H), 4.10 (q, J = 7.0 Hz, 2H), 3.82 (s, 3H), 3.08 (dd, J = 17.3 and 3.6 Hz, 1H), 2.87 (dd, J = 17.3 and 4.4 Hz, 1H), 1.18 (t, J = 7.0 Hz, 3H).

1-(4-Methoxy-phenyl)-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-3-(4-nitro-phenyl)-imidazolidine-2,4-dione (12r). R_f = 0.42 (hexane/AcOEt = 40:60); ^1H NMR (400 MHz, CDCl_3) δ 8.33 (d, J = 8.8 Hz, 2H), 7.87 (d, J = 9.1 Hz, 2H), 7.76 (d, J = 8.8 Hz, 2H), 7.20 (d, J = 9.1 Hz, 2H), 6.87 (d, J = 8.8 Hz, 2H), 6.84 (d, J = 8.8 Hz, 2H), 4.90 (dd, J = 3.7 Hz both, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 3.60 (dd, J = 17.9 and 3.7 Hz, 1H), 3.54 (dd, J = 17.9 and 3.7 Hz, 1H).; ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.4, 171.0, 164.2, 159.4, 153.6, 146.6, 138.1, 130.4, 128.7, 127.2, 126.5, 125.9, 124.0, 114.0, 113.9, 57.5, 55.5, 36.4.

1-(4-Fluoro-phenyl)-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-3-(4-nitro-phenyl)-imidazolidine-2,4-dione (12s). R_f = 0.55 (hexane/AcOEt = 50:50); ^1H NMR (400 MHz, CDCl_3) δ 8.36 (d, J = 9.0 Hz, 2H), 7.88 (d, J = 9.3 Hz, 2H), 7.83 (m, 2H), 7.22 (d, J = 8.9 Hz, 2H), 7.09 (m, 2H), 6.89 (d, J = 9.0 Hz, 2H), 4.93 (m, 1H), 3.80 (m, 1H), 3.78 (s, 3H), 3.70 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.6, 170.8, 166.0 (d, J = 256.6 Hz), 158.6, 153.5, 146.7, 138.0, 132.2 (d, J = 3.1 Hz), 130.8 (d, J = 9.4 Hz), 127.1, 126.5, 125.9, 124.4, 116.0 (d, J = 22.2 Hz), 115.0, 57.4, 55.5, 36.7, 29.7.

1-(4-Methoxy-phenyl)-3-(4-nitro-phenyl)-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (12t). R_f = 0.38 (hexane/AcOEt = 70:30); FTIR (microscope) ν 1733,

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1516 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.33 (d, $J = 8.8$ Hz, 2H), 7.56 (d, $J = 8.8$ Hz, 2H), 7.28 (d, $J = 8.8$ Hz, 2H), 7.01 (d, $J = 8.8$ Hz, 2H), 5.29 (s, 1H), 3.89 (m, 1H), 3.85 (s, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 166.6, 153.6, 146.1, 140.2, 127.5, 124.9, 124.5, 122.9, 114.8, 55.6, 55.2, 49.1 (septet, $J = 27.7$ Hz), the corresponding resonances of CF_3 groups are obscured; ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.8 (m, 3F), -64.2 (m, 3F); EIMS (m/z) 477 [M^+ (100)], 149 (62), 134 (51).

[1-Benzyl-3-(4-methoxy-phenyl)-2,5-dioxo-imidazolidin-4-yl]-acetic acid ethyl ester (13a). $R_f = 0.55$ (hexane/AcOEt = 50:50); FTIR (neat) ν 1776, 1725, 1715 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.41-7.29 (m, 7H), 6.98 (d, $J = 9.0$ Hz, 2H), 4.85 (d, $J = 15.3$ Hz, 1H), 4.42 (d, $J = 15.3$ Hz, 1H), 4.18 (dd, $J = 4.4$ Hz both, 1H), 4.08 (m, 2H), 3.83 (s, 3H), 2.92 (dd, $J = 17.1$ and 4.4 Hz, 1H), 2.83 (dd, $J = 17.1$ and 4.4 Hz, 1H), 1.19 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 171.3, 168.9, 159.4, 156.3, 135.9, 129.0, 128.2, 128.1, 127.6, 114.4, 61.3, 55.9, 55.5, 45.6, 34.2, 14.1; EIMS (m/z) 382 [M^+ (60)], 91 (100).

3-Benzyl-1-(4-methoxy-phenyl)-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (13e). $R_f = 0.54$ (hexane/AcOEt = 70:30); FTIR (neat) ν 1789, 1727, 1713 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.44 (m, 2H), 7.33 (m, 3H), 7.19 (d, $J = 8.8$ Hz, 2H), 6.94 (d, $J = 8.8$ Hz, 2H), 4.92 (s, 1H), 4.79 (d, $J = 14.2$ Hz, 1H), 4.72 (d, $J = 14.2$ Hz, 1H), 3.81 (s, 3H), 3.69 (septet, $J = 8.5$ Hz, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 167.8, 158.8, 155.0, 134.9, 129.1, 128.7, 128.3, 127.1, 126.4, 122.2 (q, $J = 279.3$ Hz), 122.0 (q, $J = 286.7$ Hz), 114.6, 55.6, 55.5, 48.6 (q, $J = 29.6$ Hz), 43.6; ^{19}F NMR (235.4 MHz, CDCl_3) δ -64.0 (quintet, $J = 8.7$ Hz, 3F), -64.5 (quintet, $J = 8.7$ Hz, 3F); EIMS (m/z) 446 [M^+ (23)], 134 (40), 91 (100).

3-Cyclohexyl-1-phenyl-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (13j). $R_f = 0.75$ (hexane/AcOEt = 80:20); ^1H NMR (400 MHz, CDCl_3) δ 7.50-7.27 (m, 5H),

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4.96 (s, 1H), 4.01 (tq, $J = 12.4$ and 3.9 Hz, 1H), 3.71 (septet, $J = 8.3$ Hz, 1H), 2.15 (m, 2H), 1.91-1.66 (m, 5H), 1.27 (m, 3H); ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.8 (quintet, $J = 8.7$ Hz, 3F), -64.5 (quintet, $J = 8.7$ Hz, 3F).

3-Benzyl-1-*tert*-butyl-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione

(13m). $R_f = 0.43$ (hexane/AcOEt = 60:40); m.p. 118-119 °C; FTIR (microscope) ν 1755, 1713, 1677, 1606 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.87 (d, $J = 9.0$ Hz, 2H), 7.41 (m, 2H), 7.28 (m, 3H), 6.93 (d, $J = 9.0$ Hz, 2H), 4.70 (d, $J = 14.5$ Hz, 1H), 4.63 (d, $J = 14.5$ Hz, 1H), 4.57 (dd, $J = 6.2$ and 2.8 Hz, 1H), 3.86 (s, 3H), 3.61 (dd, $J = 17.6$ and 6.2 Hz, 1H), 3.42 (dd, $J = 17.6$ and 2.8 Hz, 1H), 1.42 (s, 9H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.5, 173.0, 163.9, 156.7, 136.4, 130.4, 129.4, 128.5, 127.6, 113.9, 55.5, 42.4, 40.6, 28.6; EIMS (m/z) 395 [$\text{M}^+ + 1$ (11)], 394 [M^+ (19)], 338 (40), 203 (64), 135 (46), 91 (100).

3-Benzyl-1-*tert*-butyl-5-[2-(4-fluoro-phenyl)-2-oxo-ethyl]-imidazolidine-2,4-dione (13n).

$R_f = 0.48$ (hexane/AcOEt = 60:40); m.p. 123-25 °C; FTIR (microscope) ν 1754, 1705 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 7.90 (m, 2H), 7.39 (m, 2H), 7.34-7.24 (m, 3H), 7.12 (m, 2H), 4.68 (d, $J = 14.5$ Hz, 1H), 4.60 (d, $J = 14.5$ Hz, 1H), 4.55 (dd, $J = 6.2$ and 2.8 Hz, 1H), 3.60 (dd, $J = 17.6$ and 6.2 Hz, 1H), 3.44 (dd, $J = 17.6$ and 2.8 Hz, 1H), 1.42 (s, 9H); ^{13}C NMR (62.9 MHz, CDCl_3) δ 193.5, 172.8, 166.1 (d, $J = 257.1$ Hz), 156.7, 136.2, 132.8, 130.7 (d, $J = 9.2$ Hz), 128.6, 127.7, 127.4, 115.9 (d, $J = 22.2$ Hz), 55.7, 55.4, 42.4, 40.8, 28.6; ^{19}F NMR (235.4 MHz, CDCl_3) δ -105.1 (m, 1F); EIMS (m/z) 382 [M^+ (45)], 91 (100).

2-[1-(4-Methoxy-phenyl)-3-(4-nitro-phenyl)-2,5-dioxo-imidazolidin-4-yl]-malonic acid diethyl ester (13p). $R_f = 0.35$ (hexane/AcOEt = 70:30); FTIR (microscope) ν 1734 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.33 (d, $J = 8.5$ Hz, 2H), 7.81 (d, $J = 8.5$ Hz, 2H), 7.26 (d, $J = 9.0$ Hz, 2H), 6.97 (d, $J = 9.0$ Hz, 2H), 5.16 (d, $J = 3.9$ Hz, 1H), 4.32 (m, 2H), 4.16 (m, 2H), 3.94 (d, $J = 3.9$ Hz,

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1H), 3.83 (s, 3H), 1.31 (t, $J = 7.1$ Hz, 3H), 1.19 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 168.5, 165.7, 165.4, 158.9, 153.3, 146.8, 137.6, 126.5, 126.4, 126.2, 124.4, 115.1, 62.8, 62.4, 59.7, 55.7, 51.4, 13.9; EIMS (m/z) 486 [$\text{M}^+ + 1$, (56)], 366 (100).

[1-(4-Methoxy-phenyl)-3-(4-nitro-phenyl)-2,5-dioxo-imidazolidin-4-yl]-acetic acid ethyl ester (13q). $R_f = 0.19$ (hexane/AcOEt = 70:30); FTIR (microscope) ν 1723, 1516 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.28 (d, $J = 9.3$ Hz, 2H), 7.66 (d, $J = 9.3$ Hz, 2H), 7.37 (d, $J = 9.0$ Hz, 2H), 7.00 (d, $J = 9.0$ Hz, 2H), 4.94 (dd, $J = 4.9$ and 3.4 Hz, 1H), 4.10 (m, 2H), 3.84 (s, 3H), 3.18 (dd, $J = 17.6$ and 3.4 Hz, 1H), 3.02 (dd, $J = 17.6$ and 4.9 Hz, 1H), 1.16 (t, $J = 7.2$ Hz, 3H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 169.7, 168.4, 159.8, 154.0, 144.4, 141.3, 127.8, 125.1, 123.9, 120.8, 114.6, 61.6, 55.9, 55.5, 33.0, 14.0; EIMS (m/z) 413 [M^+ (100)], 339 (69), 149 (60).

3-(4-Methoxy-phenyl)-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-1-(4-nitro-phenyl)-imidazolidine-2,4-dione (13r). $R_f = 0.42$ (hexane/AcOEt = 40:60); FTIR (microscope) ν 1723, 1515 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.22 (d, $J = 8.3$ Hz, 2H), 7.79 (d, $J = 8.5$ Hz, 2H), 7.67 (d, $J = 8.5$ Hz, 2H), 7.46 (d, $J = 8.5$ Hz, 2H), 7.03 (d, $J = 8.5$ Hz, 2H), 6.87 (d, $J = 8.3$ Hz, 2H), 5.13 (m, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.78 (m, 1H), 3.63 (m, 1H); ^{13}C NMR (100.6 MHz, CDCl_3) δ 192.9, 170.6, 164.3, 159.8, 154.2, 144.2, 141.5, 130.4, 128.6, 128.0, 125.1, 124.1, 121.0, 114.7, 114.0, 55.9, 55.5, 36.3; EIMS (m/z) 475 [M^+ (16)], 340 (100), 135 (55).

3-(4-Fluoro-phenyl)-5-[2-(4-methoxy-phenyl)-2-oxo-ethyl]-1-(4-nitro-phenyl)-imidazolidine-2,4-dione (13s). $R_f = 0.55$ (hexane/AcOEt = 50:50); FTIR (microscope) ν 1721, 1516 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.26 (d, $J = 9.1$ Hz, 2H), 7.86 (m, 2H), 7.68 (d, $J = 9.1$ Hz, 2H), 7.45 (d, $J = 9.1$ Hz, 2H), 7.09 (m, 2H), 7.04 (d, $J = 9.1$ Hz, 2H), 5.14 (dd, $J = 4.0$ and 3.0 Hz, 1H), 3.85 (s, 3H), 3.78 (dd, $J = 18.2$ and 4.0 Hz, 1H), 3.69 (dd, $J = 18.2$ and 3.0 Hz); ^{13}C NMR (100.6 MHz, CDCl_3) δ 193.0, 170.4, 166.2 (d, $J = 256.9$ Hz), 159.9, 154.2, 144.3, 141.3, 132.0 (d, J

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= 3.1 Hz), 130.8 (d, $J = 9.6$ Hz), 128.0, 125.2, 124.0, 120.9, 116.1 (d, $J = 22.4$ Hz), 114.7, 55.7, 55.6, 36.5, 29.7; ^{19}F NMR (235.4 MHz, CDCl_3) δ -103.7 (m, 1F); EIMS (m/z) 464 [$\text{M}^+ + 1$ (17)], 463 [M^+ (23)], 340 (100).

3-(4-Methoxy-phenyl)-1-(4-nitro-phenyl)-5-(2,2,2-trifluoro-1-trifluoromethyl-ethyl)-imidazolidine-2,4-dione (13t). $R_f = 0.43$ (hexane/AcOEt = 70:30); FTIR (microscope) ν 1733, 1516 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 8.34 (d, $J = 9.0$ Hz, 2H), 7.57 (d, $J = 9.0$ Hz, 2H), 7.27 (d, $J = 9.0$ Hz, 2H), 7.01 (d, $J = 9.0$ Hz, 2H), 5.28 (s, 1H), 3.87 (m, 1H), 3.84 (s, 3H); ^{13}C NMR (400 MHz, CDCl_3) δ 166.6, 160.2, 153.6, 146.2, 140.3, 127.5, 124.8, 124.5, 123.1, 122.3 (q, $J = 281.2$ Hz), 122.2 (q, $J = 282.3$ Hz), 55.6, 55.3, 49.3 (septet, $J = 28.8$ Hz); ^{19}F NMR (235.4 MHz, CDCl_3) δ -63.7 (m, 3F), -64.1 (m, 3F); EIMS (m/z) 477 [M^+ (78)], 149 (100), 134 (56).