Supplementary Material

Facile Domino Access to Unexpected Alkyl 3-Substituted-2-Hydroxy-3,4-Dihydro-2H-1,4-Benzoxazine-2-Carboxylates

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1. General Methods:

NMR spectra were recorded with tetramethylsilane as the internal standard. TLC was performed on glass-backed silica plates. Column chromatography was performed using silica gel (160-200 mesh) eluting with ethyl acetate and petroleum ether. 

$^1$H NMR spectra were recorded at 400 MHz, and $^{13}$C NMR spectra were recorded at 100 MHz (Bruker Avance). Chemical shifts (δ) are reported in ppm downfield from CDCl$_3$ (δ = 7.26 ppm) for $^1$H NMR and relative to the central CDCl$_3$ resonance (δ = 77.0 ppm) for $^{13}$C NMR spectroscopy. Coupling constants (J) are given in Hz. ESI-HRMS spectrometer was measured with a Finnigan LCQ DECA ion trap mass spectrometer.

2. X-ray data of 3aa

Crystal data for 3aa C$_{13}$H$_{15}$NO$_5$ (265.26), Triclinic, space group P-1, $a = 5.8989(4)$ Å, $b = 9.2987(6)$ Å, $c = 13.0803(9)$ Å, $V = 695.86(8)$ Å$^3$, $Z = 2$, specimen 0.251 x 0.0175 x 0.121 mm$^3$, $T = 296(2)$ K, SIEMENS P4 diffractometer, absorption coefficient 0.098 mm$^{-1}$, reflections collected 11416, independent 3210 [R(int) = 0.0222], refinement by Full-matrix least-squares on $F^2$, data/restraints/parameters 3210 / 0 / 173, goodness-of-fit on $F^2 = 1.038$, final $R$ indices [$I>2\sigma(I)$] R1 = 0.0459, wR2 = 0.1413, $R$ indices (all data) R1 = 0.0545, wR2 = 0.1497, largest diff. peak and hole 0.602 and - 0.509 Å$^{-3}$. 

Molecular Structure of 3aa (ellipsoids with 50% probability)
3. $^1$H NMR and $^{13}$C NMR spectra
3ab
3ac
3da