An Unexpected Three Component Condensation Leading to Amino(3-oxo-2,3-dihydro-1*H*-isoindol-1-ylidene)acetonitriles

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General Experimental Methods. All reactions were carried out under an inert atmosphere of argon unless stated otherwise. Methanol was dried with magnesium and distilled. Analytical TLC was performed on aluminium backed TLC-plates coated with aluminium oxide N/UV₂₅₄. Compounds were visualized by UV light (254 nm) and by dipping the plates in alkaline KMnO₄ solution and heating. Flash chromatography was performed on silica gel (40–63 μ m). Chemical shifts were referenced to the residual solvent peak (DMSO-*d*₆, δ_{H} = 2.50 ppm, $\delta_{\text{C, central}}$ = 39.43 ppm; CDCl₃, δ_{H} = 7.24 ppm, $\delta_{\text{C, central}}$ = 77.0 ppm). Coupling constants were determined via Lorentz-Gauss transformation. ¹³C NMR spectra were recorded with ¹H broad band decoupling; if necessary, signals were assigned based on DEPT-135, gs-COSY-90, gs-HMQC, and gs-HMBC spectra. ESI-MS spectra were measured in acetonitrile/water 70:30 at a cone voltage of 70V. FD-MS spectra were recorded at a desorption voltage of 5 kV and a heater current of 10 mA/min. Melting points were measured on a Dr. Tottoli apparatus and are uncorrected. Except for compounds **5** and (Z)-**7d**, the products did not have melting points but rather started decomposing at the given temperatures.

Compound **5**: ^1H NMR (300 MHz, $\text{DMSO-}d_6$)

Compound **5**: ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$)

Compound **7a**: ^1H NMR (300 MHz, $\text{DMSO-}d_6$)

Compound **7a**: ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$)

Compound (Z)-**7a** (still contains small amounts of the *E*-isomer): ^1H NMR (400 MHz, $\text{DMSO-}d_6$)

Compound (Z)-**7a** (still contains small amounts of the *E*-isomer): ¹³C NMR (75.5 MHz, DMSO-*d*₆)

Compound (E)-**7b**: ¹H NMR (300 MHz, DMSO-*d*₆)

Compound (E)-7b: ^{13}C NMR (75.5 MHz, DMSO- d_6)

Compound (Z)-**7b**: ¹H NMR (300 MHz, DMSO-*d*₆)

Compound (Z)-7b: ¹³C NMR (75.5 MHz, DMSO-*d*₆)

Compound (E/Z)-7c: ¹H NMR (300 MHz, DMSO-*d*₆)

Compound (*E/Z*)-**7c**: ¹³C NMR (75.5 MHz, DMSO-*d*₆)

Compound (E/Z)-7d: ^1H NMR (300 MHz, $\text{DMSO}-d_6$)

Compound (E/Z)-**7d**: ^{13}C NMR (75.5 MHz, DMSO- d_6)

Compound (Z)-7d: ^1H NMR (300 MHz, $\text{DMSO}-d_6$)

Compound (Z)-**7d**: ¹³C NMR (75.5 MHz, DMSO-*d*₆)

Compound (Z)-7f: ^{13}C NMR (75.5 MHz, DMSO- d_6)

Compound (E)-7g: ^1H NMR (300 MHz, $\text{DMSO}-d_6$)

Compound (E)-7g: ^{13}C NMR (75.5 MHz, DMSO- d_6)

Compound (Z)-7g: ^1H NMR (300 MHz, $\text{DMSO}-d_6$)

Compound (Z)-7g: ^{13}C NMR (75.5 MHz, $\text{DMSO}-d_6$)

Compound (Z)-7h: ^1H NMR (300 MHz, DMSO- d_6)

Compound (Z)-7h: ^{13}C NMR (75.5 MHz, DMSO- d_6)