Experiment id : 3 (PRODUCER : null (id:0))

REACTANTS TABLE:

amount	condition	equality	formula	id	moles	mw	name
186.008	solid	1.0	C₆H₄BrNO	3	1.0	186.01	5-bromonicotinaldehyde

REAGENTS TABLE:

amount	condition	equality	formula	id	moles	mw	name
84.162	solid	1.0	C₆H₁₂	3	1.0	84.16	cyclohexane

PRODUCTS TABLE:

amount	condition	equality	formula	id	moles	mw	name
208.006	crude	1.0	C₆H₄BrF₂N	3	1.0	208.01	3-bromo-5-(difluoromethyl)pyridine

PROCEDURE:

Starting materials 1a-h, 1k-1y, 2a-p as well as solvents for the reactions, were acquired from commercial sources (tetrahydrofuran was inhibitor free, water was tab water). Starting materials 1i, 1j and 10 were synthesized following a procedure described in the literature.1 For thin layer chromatography (TLC), silica gel plates with fluorescence indicator 254 nm were used and compounds were visualized by irradiation with UV light and/or by treatment with a solution of potassium permanganate in water followed by heating. Flash column chromatography was performed using Geduran® Silica Gel 60 (0.040-0.063 nm). Cyclohexane, ethyl acetate, dichloromethane and methanol for flash chromatography were acquired from commercial sources and were used without previous purification. NMR spectra were acquired on a Bruker Avance 300 MHz spectrometer, running at 300 and 75 MHz for 1H and 13C, respectively. 19F-NMR spectra were acquired on a Bruker Avance 500 MHz spectrometer, running at 471 MHz. Chemical shifts (δ) are reported in ppm relative to residual solvent signals (CDCl3, 7.26 ppm for 1H-NMR and 77.2 ppm for 13C-NMR). 13C-NMR was acquired on a broad band decoupled mode. The following abbreviations are used to describe peak patterns when appropriate: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), m (multiplet), bs (broad singlet), tt (triplet of triplets), td (triplet of doublets). Electrospray ionization has been used for measuring the exact mass (indicated for each case): MS (ESI) (Electrospray ionization mass spectroscopy) was acquired with an Agilent Technologies 6120 Quadrupole LC/MS. In this technique, MassWorks software ver. 4.0.0.0 (Cerno Bioscience) was used for the formula identification. MassWorks is a MS calibration software which calibrates for isotope profile as well as for mass accuracy, allowing highly accurate comparisons between calibrated and theoretical spectra.2