Supporting Information

Synthesis of novel pyrazole-based heterocycles via a copper(II)-catalysed domino annulation

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I. General Remarks

¹H NMR and ¹³C NMR spectras were recorded in DMSO-d₆ and CDCl₃, using a Bruker Avance-500 NMR spectrometer. Chemical shifts (in ppm) were referenced to tetramethylsilane ($\delta = 0$ ppm) in DMSO-*d*₆ as an internal standard.¹³C NMR spectras were calibrated with DMSO- d_6 ($\delta = 39.57$ ppm). ¹H NMR data are reported as follows: chemical shift (δ , ppm), multiplicity (s = singlet, d = doublet, t = triplet, q= quartet, m = multiplet, bs = broken singlet, broad s = broad singlet), coupling constants (J) and assignment. Data for ¹³C NMR are reported in terms of chemical shift (δ , ppm). Mass spectras were recorded by means of a triple quadrupole mass spectrometer in ES positive mode. Elemental analyses were performed using a Perkin-Elmer 2400 elementary analyzer. Melting points are uncorrected. Reactions were monitored by thin-layer chromatography (TLC) on TLC Silica Gel 60 F₂₅₄. Chromatograms were displayed by fluorescence quenching with UV light at 254 nm, flash chromatography purifications were carried out using Silica Gel (particle size 0.040-0.063 mm). Microwave-aided experiments were performed by using a CEM DiscoverTM Microwave System. All chemicals and solvents were of commercial grade and used without further purification. Starting materials **1a-i** were synthetized according to the literature,^[1] completing the purification procedure with flash chromatography by means of an Teledyne Isco CombiFlash® Rf equipment (eluent: n-hexane/EtOAc gradient) and subsequent crystallisation from Et₂O.

^[1] L. H. Pettus, R. P. Wurz, S. Xu, B. Herberich, B. Henkle, Q. Liu, H. J. McBride, S. Mu, M. H. Plant, C. J. M. Saris, L. Sherman, L. M. Wong, S. Chmait, M. R. Lee, C. Mohr, F. Hsieh, A. S. Tasker, *J. Med. Chem.*, 2010, 53, 2973.



















































































8.0094 8.0229 8.1802 9,5030 7,33114 7,52111 7,5575211 7,5875364 6500364 4,4109 4,4230 4,4352 4,0174 4,0296 4,0417 CI N 9a PPM 9.2 8.8 8.4 8.0 7.6 7.2 6.8 6.4 6.0 5.6 5.2 4.8 4.0 4.4





