

Spectroscopic Information for Key compounds and advanced intermediates

For detailed experimental procedures for the synthesis of all compounds along with spectral information please see: Liras, Spiros; McHardy, Stanton Furst “*Preparation of 4-phenyl-4-heteroaryl piperidines as ligands for opioid receptors*” Jpn. Kokai Tokkyo Koho, (2000) JP 2000247969

Specific examples in the paper:

Compound 2: $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.72 (s, 2H), 7.05 (app t, 1H), 6.78-6.90 (comp, 2H), 6.55-6.62 (m, 1H), 3.54-3.63 (comp, 2H), 3.20-3.28 (comp, 2H), 2.61-3.05 (comp, 5H), 2.02-2.58 (comp, 5H), 1.75-1.81 (m, 1H), 1.1.05-1.39 (comp, 10H), 0.78-0.92 (comp, 6H); MS (M+1) 439.3

Compound 12: $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.71 (s, 2H), 7.89 (t, $J=1.95$ Hz, 1 H), 7.53-7.60 (m, 1 H), 7.42 - 7.49 (m, 1 H), 7.27 - 7.34 (m, 1 H), 6.38 (br. s., 1H), 5.75 (br. s., 1H) 3.44 - 3.57 (m, 2 H), 3.26 (br. s., 2H), 3.01-3.10 (comp, 2H), 2.88-2.99 (comp, 2H), 2.45-2.59 (comp, 2H), 2.16 - 2.28 (comp, 4 H), 1.65-1.75 (m, 1H), 1.15-1.39 (comp, 9H), 1.01-1.14 (m, 1H), 0.89 (d, $J=6.64$ Hz, 3 H), 0.84 (t, $J=7.13$ Hz, 3 H); MS (M+1) 466.3

Compound 9: 2-[1-allyl-1-(3-methoxyphenyl-but-3-enyl)pyrimidine-5-carboxylic acid methyl ester $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 9.19 (s, 2H), 7.16 (app t, 1H), 6.68-6.73 (comp, 3H), 5.36-5.46 (comp, 2H), 4.91-5.01 (comp, 4H), 3.92 (s, 3H), 3.72 (s, 3H), 3.04-3.71 (comp, 4H); MS (M+1) 339.3

Compound 10: 2-[1-benzyl-4-(3-methoxy-phenyl)-piperidin-4-yl]-pyrimidine-5-carboxylic acid methyl ester $^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.72 (s, 2H), 7.14-7.29 (comp, 6H), 6.95-6.97 (comp, 2H), 6.65-6.68 (m, 1H), 3.73 (s, 3H), 3.52-3.54 (comp, 2H), 3.39 (s, 2H), 3.25-3.27 (comp, 2H), 2.95-2.98 (comp, 2H), 2.74-2.77 (comp, 2H), 2.31-2.34 (comp, 2H), 2.02-2.16 (comp, 2H), 1.17-1.26 (comp, 6H); MS (M+1) 459.2