

4-{[(3,5-dimethyl-1*H*-pyrazol-1-yl)methyl]amino}benzoic acid

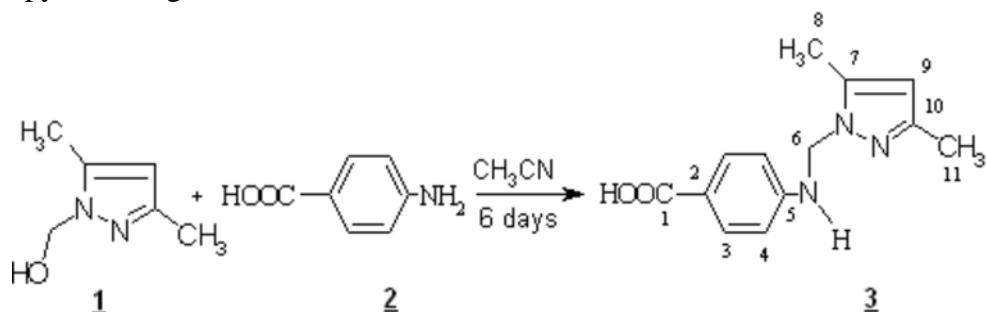
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A mixture of (3,5-dimethyl-1*H*-pyrazol-1-yl)methanol **1** [1] (1.84 g, 14.6 mmol) and 4-aminobenzoic acid **2** (1g, 7.3 mmol) in acetonitrile (50 mL) was stirred in a closed vessel at room temperature for 6 days [2, 3, 4]. The white precipitate was filtered off, washed with acetonitrile and dried in air. Yield: (1.54g, 68.5%).

Melting Point = 210-212°C (CH₃CN).

IR (KBr, cm⁻¹): 3260(s, NH), 3140, 3100, 3040, 3000, 2840, 2700, 2620, 1700(s, C=O), 1600 (s, C=C), 1550(s, C=N), 1420(s, C-N), 1260(s, -C-OH), 1150(s).

¹H NMR (400 MHz, DMSO-d₆) δ ppm: 7.63 (d, 2H, Ph, J= 5.71 Hz); 7.35 (t, 1H, -NH, J= 3.42Hz); 6.8 (d, 2H, Ph, J= 5.71 Hz); 5.7 (s,1H, Pz); 5.25 (d, 2H, N-CH₂- N, J=3.42 Hz); 2.22(s, 3H, CH₃); 1.95(s, 3H, CH₃).

¹³C NMR (100 MHz, DMSO-d₆) δ ppm: 167.51(C1), 150.91(C5), 145.65(C3), 138.71(C2), 131.02(C4), 118.95(C7), 112.04(C10), 105.47(C9), 56.39(C6), 13.42(C8), 10.75(C11).

FAB MS: 246[M+1].

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Sample Availability: Available from the Authors.

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