Synthesis of methyl N’-[1-(4-hydroxybutyl)-3-(trifluoromethyl)-1H-1,2,4-triazol-5-yl]-N-phenylimidothiocarbamate

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The desired compound 2 was obtained by complete deacetylation of compound 1 [1] using triethylamine [2]. To a solution of 1 (0.623g, 1.5 mmol) in methanol (15 ml) was added triethylamine (2 ml). The mixture was stirred at room temperature and the reaction was followed by TLC. After complete deacetylation (24 hours), the reaction mixture was evaporated and coevaporated with methanol (3x30 ml) under reduced pressure, then chromatographed over silica gel using CH₂Cl₂/MeOH (98:2 v/v) to give compound 2 as white powder crystallized from n-Hexane/ Ethylacetate.

Melting point: 113-114 ºC.

Elemental Analysis: Calculated for C₁₅H₁₈F₃N₅SO: C, 48.26%; H, 4.83%; N, 18.77%. Found: C, 48.35%; H, 4.98%; N, 18.75%.

UV (EtOH, λ_max): 277nm

IR (KBr, cm⁻¹): 3448 (OH group)

MS (m/z): 374 (M⁺)

¹H-NMR (250 MHz, DMSO): δ= 1.7(m,2H,HOCH₂CH₂); 2.1(m,2H, CH₂CH₂-N); 2.1 (s,3H,SCH₃); 3.7(t,2H,OCH₂ ); 4.3 (m,2H,NCH₂); 4.8(m,1H,OH, D₂O exchangeable); 7.6-7.8 (m,5H, aromatic).

References
Sample Availability: Available from MDPI.

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