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Research Article

Multi-step Synthesis and Characterization of novel 6-(2,6-dimethoxypyrimidin-4-yl)-4-methoxy-1-(2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)ethyl)-1*H*-benzo[d]imidazolescaffold

Srikanth Podishetty [1], Shabhari Prasad Suggala[2], Jagadeesh Kumar Ega [1*]

Corresponding Author:
jkjagadeeshkumare@gmail.com

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ABSTRACT

At first5-bromo-1-fluoro-3-methoxy-2-nitrobenzene 2 formed from a stirred solution of 5-bromo-1, 3-difluoro-2-nitrobenzene 1 MeOH/ KOH to give ether via NPSRN. Compound 2 treated withtert-butyl (2-aminoethyl) carbamate under THF to yield Boc protected tert-butyl (2-((5-bromo-3-methoxy-2-nitrophenyl) amino) ethyl) carbamate 3.It is further with Zn dustNH4Cl under THF/H2O to give tert-butyl (2-((2-amino-5-bromo-3-methoxyphenyl) amino) ethyl) carbamate 4 through reduction. It is further interacted with triethyl orthoformate, PTSA catalytic amount to yield tert-butyl (2-(6-bromo-4-methoxy-1H-benzo[d]imidazol-1-yl) ethyl) carbamate 5 via cyclization. Furthermore, with Bis (pina-colato) diborane under dry Dioxane and PdCl2 (dppf)/ DCM to yield tert -butyl (2-(4-methoxy-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-benzo[d]imidazol-1-yl)ethyl) carbamate 6. Compound 6 charged with4-bromo-2,6-dimethoxypyrimidine followed by PdCl2 (dppf) CH2Cl2 to give tert-butyl (2-(6-(2,6-dimethoxypyrimidin-4-yl)-4-methoxy-1H-benzo[d]imidazol-1-yl) ethyl) carbamate 7 through cross coupling. It is interacted with BBr3 which acts as Lewis acid under DCM to form 6-(1-(2-aminoethyl)-4-hydroxy-1H-benzo[d]imidazol-6-yl) pyrimidine-2, 4(1H, 3H)-dione hydrochloride 8. Then reaction mixture is charged witht-BuONO followed by 1.77 mmol TMSN3 drop-wise under CH3CN to give desired azide namely 1-(2-azidoethyl)-6-(2, 6-dimethoxypyrimidin-4-yl)-4-methoxy-1H-benzo[d]imidazole 9. Finally,label compound 9 under goes 3+2 cyclo addition with Phenyl acetylene in the presence of CuSO4.5H2O/ sodium ascorbate familiarly Sharpless catalyst which convert Cu (II) to Cu(I) during the course of the reaction to yield target 6-(2,6-dimethoxypyrimidin-4-yl)-4-methoxy-1-(2-(4-phenyl-1H-1,2,3-triazol-1-yl)ethyl)-1H-benzo[d]imidazole 10 with an excellent yields depicted (Scheme I) in this manuscript viz click protocols.

Keywords: Boc protection, pyrimidine, benzo[d]imidazole, 1, 2, 3-triazole, Cyclization, PdCl2 (dppf), BBr3, TMSN3, 3+2 cyclo addition, coupling, deprotection.

[1, 2, 1*] Chaitanya (Deemed to be University), (V) Himayathnagar, (M)Moinabad, (District) Ranga Reddy, Hyderabad -500075, Telangana, India.

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