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Synthesis of new derivatives of a novel [1,3]selenazolo[5,4-*e*][1,2,4]triazolo[1,5-*c*]pyrimidine heterocyclic architecture via Dimroth rearrangement

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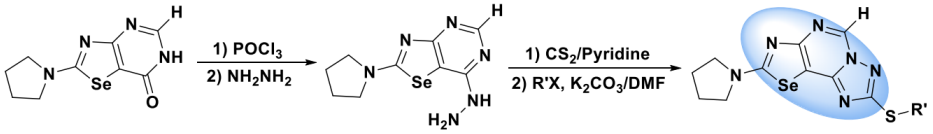
Amongst heterocyclic organoselenium cores, 1,3-selenazole skeleton has received much attention from medicinal chemists. The worldwide high profile of 1,3-selenazoles is not only because of the presence of the selenazole moiety in many pharmacologically active substances such as selenazofurin and amselamine, but also biological properties include antioxidant [1], anticancer [2], human carbonic anhydrase IX inhibitory [3], antimicrobial and anticonvulsant [4] activities. Based on the broad spectrum biological activities of selenazoles and aiming to synthesize novel fused heterocycles containing Se in their scaffold, in the present protocol, 2-(pyrrolidin-1-yl)-[1,3]selenazolo[4,5-*d*]pyrimidin-7(6*H*)-one **(1)** was synthesized as a starting material and subsequently treated with $POCl_3$ and hydrazine hydrate to give 7-hydrazinated selenazolo[4,5-*d*]pyrimidines **(2)**. The heterocyclization of compound **(2)** with CS_2 via pyridine base-catalyzed Dimroth rearrangement yielded a novel tricyclic [1,3]selenazolo[5,4-*e*][1,2,4]triazolo[1,5-*c*]pyrimidine framework which was subsequently converted to the desired *S*-alkylated derivatives **(3a-f)** on treatment with various alkyl halides in the presence of K_2CO_3/DMF in good yields.



(6a): R'= Me; (6b): R'= Et; (6c): R'= *n*-Pr; (6d): R'= *n*-Bu; (6e): R'= Bn; (6f): R'= CH_2CO_2Et

Keywords: Selenazole, [1,3]selenazolo[5,4-e][1,2,4]triazolo[1,5-c]pyrimidine, Base-catalyzed Dimroth rearrangement, Selenazolo[4,5-d]pyrimidine

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