Abstract

Heterocyclic compounds have a significant position in organic especially *pharmaceutical industry due to their immense and diverse properties. The present* research attempted to create a unique heterocyclic unit since the chemistry of synthesized compounds have gained ample importance. The synthesized compound entailed different functional group including azacyclohexane ring, sulfonamide moiety and 1,2,4-triazole nucleus named as 5-{1-[(4-methoxy phenyl)sulfonyl]-4-piperidinyl}-4-methyl-4*H*-1,2,4-triazole-3-thiol (6). The multistep syntheses route was adopted to generate the designed compound through four consecutives steps. First ethyl 1-[(4-methoxy phenyl)sulfonyl]piperidine-4-carboxylate (3) was developed by reacting ethyl isonipecotate (1) and 4-methoxybenzene sulfonyl chloride (2), the carboxylate group of product (3) was transferred into hydrazide by treating with hydrazine resulting in formation of 1-[(4-methoxy phenyl)sulfonyl]piperidine-4-carbohydrazide (4). The final cyclization of compound (5) 1,2,4-triazole nucleus takes place at last step upon adding methyl isothiocyanate in product (4) and providing suitable conditions. A two *S*-substituted 3-aralkylthio-5-{1-[(4-methoxy phenyl)sulfonyl]-4-piperidinyl}-4-methyl-4*H*-1,2,4-triazole derivatives were also produced by keeping the mixture of electrophiles and compound (5) under conventional as well as microwave environment. The structural elucidation of prepared compounds was done using IR, ^{1}H-NMR and ^{13}C-NMR spectra whereas the aralkyl derivatives were screened through three enzymatic assays to evaluate their biological proficiency. The results of acetylcholinesterase (AChE), lipoxygenase (LOX) and bovine serum albumin (BSA) activity revealed that all derivatives exhibit potential against tested enzymes. Molecular docking studies were made to get the in-depth knowledge and visualize the binding interactions of synthesized compounds with respective enzymes.