

Abstract

Heterocyclic compounds indissolubly woven into the processes of life. Pharmaceutical industries has showed vital interest in heterocycles. Organic chemistry has abundance of heterocyclic systems through synthesis. Heterocycles have attained much attention in medicinal chemistry as they exhibit various valuable biological potential. Pharmaceutical industries are flourishing day-by-day by opting eco-friendly and economic methodologies. We here selected four exceedingly significant motif which are well-known pharmacophores i.e., imidazoles, pyrazoles, oxadiazole, triazole. Emphasis was given to promote the green synthesis, mostly by designing solvent-free reactions, introducing inexpensive catalyst, using precursors those are nontoxic and synthesizing bioactive compounds. For method development pyridine-2-carboxylic acid was selected as organo-catalyst to explore its catalytic potential, good to excellent yields of 2,4,5-triphenyl imidazoles were obtained. Optimized conditions and the proposed mechanism involved in the condensation reaction was discussed in chapter 4. Biological potential of 2,4,5 triphenyl imidazoles was evaluated against anti-urease and AChE inhibition activity. 4-(4,5-diphenyl-1H-imidazol-2-yl)-2-ethoxyphenol (**227m**) proved most potent candidate against AChE inhibition activity and molecular docking also support this data. 2-(4-bromophenyl)-4,5-diphenyl-1H-imidazole (**227j**) exhibited greater positive response against anti-urease activity.

4-Hydroxybenzene 1,3-dicarboxylic acid was selected for carrying out series of reactions. 4-Hydroxybenzene 1,3-dicarbohydrazide (**230**) and its derivatives were synthesized and explored their potential against different biological activities. The synthetic **scheme 2.36** depicted the synthesis of novel hydrazones by the reaction of hydroxybenzene 1,3-dicarbohydrazide (**230**) with selected aromatic aldehydes in ethanol. 4-hydroxy-N³-[(Z)-1H-indol-3-ylmethylidene]-N¹-[(E)-1H-indol-3-ylmethylidene] benzene-1,3-dicarbohydrazide (**231e**) proved good candidate drug for Alzheimer disease (AD) because it showed activity against both AChE and BChE inhibition. N¹-[(E)-(4-chlorophenyl) methylidene]-N³-[(Z)-(4-chlorophenyl) methylidene]-4-hydroxybenzene-1,3-dicarbohydrazide (**231h**) evaluated as potent anti-urease agent. The compounds synthesized through this series screened against DPPH antioxidant activity. 4-hydroxy-N¹-[(E)-(4-hydroxy-3-ethoxyphenyl)methylidene]-N³-[(Z)-(4-hydroxy-3-xviii

ethoxyphenyl)methylidene)methylidene]benzene-1,3-dicarbohydrazide (**231d**) proved good antioxidant. In **scheme 2.37** novel compound 2,2'-[(4-hydroxybenzene-1,3-diyl)dicarbonyl] bis(5-methyl-2,4-dihydro-3H-pyrazol-3-one) (**233**) was synthesized by the reaction of hydroxybenzene 1,3-dicarbohydrazide with ethylacetoacetate in solvent-free environment by heating reactants and these were further derivitized by reacting 2,2'-[(4-hydroxybenzene-1,3-diyl)dicarbonyl] bis(5-methyl-2,4-dihydro-3H-pyrazol-3-one) with selected aromatic aldehydes. 2,2'-[(4-hydroxybenzene-1,3-diyl)dicarbonyl]bis(4-hydroxybenzylidene-5-methyl-2,4-dihydro-3H-pyrazol-3-one) (**234b**) showed good activity against AChE and BChE and 2,2'-[(4-hydroxybenzene-1,3-diyl)dicarbonyl]bis(2,4-dihydroxybenzylidene-5-methyl-2,4-dihydro-3H-pyrazol-3-one) (**234d**) against antioxidant activity. In **scheme 2.38** compound **230** was refluxed with ethylisocyanate in ethanol and 10% NaOH was used for cyclization and [5-(4-Ethyl-5-mercapto-4H-[1,2,4]triazole-3-carbonyl)-2-hydroxy-phenyl]-(4-ethyl-5-mercapto-4H-[1,2,4]triazol-3-yl)-methanone (**236**) was formed. Biological potential of this novel compound was determined against AChE and BChE and it proved potent against AChE. In **scheme 2.39** compound **230** was used to synthesize [2-hydroxy-5-(5-mercapto-[1,3,4]oxadiazole-2-carbonyl)-phenyl]-(5-mercapto[1,3,4] oxadiazol-2-yl)-methanone (**237**) by refluxing in ethanol with CS₂ and KOH. Moreover the molecular docking studies were also carried out for the enhancing the understanding of structure-activity relationship.