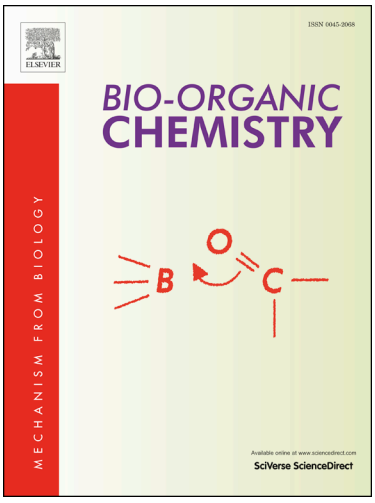

Modification of Bischler-Möhlau Indole Derivatives through Palladium Catalyzed Suzuki Reaction as Effective Cholinesterase Inhibitors, their Kinetic and Molecular Docking Studies

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Modification of Bischler-Möhlau Indole Derivatives through Palladium Catalyzed Suzuki Reaction as Effective Cholinesterase Inhibitors, their Kinetic and Molecular Docking Studies

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Abstract: Due to the immense importance of aryl indole nucleus, herein we report the palladium-catalyzed arylation of *N*-substituted 2-aryl indole utilizing Suzuki-Miyaura cross coupling methodology. The biological screening for cholinesterase inhibition of the resulted biaryl indole moieties was carried out to evaluate their pharmacological potential, expecting to involve the development of new therapeutics for various inflammatory, cardiovascular, gastrointestinal and neurological diseases. This research work also involved the use of utilization of microwave-assisted organic synthesis (MAOS) for the synthesis of Bischler-Möhlau indole which is further biarylated *via* palladium-catalyzed cross coupling reaction. All the synthetic compounds (**3a-n**) were tested for cholinesterase inhibition and exhibited high level of AChE inhibitory activities. Interestingly, compounds **3m** and **3n** were found to be dual inhibitors, however, remaining compound exhibited no any inhibitory activity against BChE. The biological potential of the resulted compounds was explained on the basis of molecular docking studies, performed against AChE and BChE, exploring the probable binding modes of most potent inhibitors.

Keywords: Biaryl indole moieties, Cholinesterase, Molecular docking, Palladium-catalyzed, Suzuki-Miyaura Cross Coupling

Introduction:

Cholinesterases (ChEs), members of serine hydrolase family of enzymes, play important roles in the termination of acetylcholine based signal transmission through neurosynaptic cleft.[1-2] In

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