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Title of the thesis: **"Studies Towards Synthesis and Efficacy of New Heterocyclic Scaffolds and Zwitter Ionic Molecules"**

ABSTRACT:

The thesis contains four chapters including a general introduction as the first chapter and three other chapters. The second chapter addresses a problem of rotational isomers observed in the case of tertiary amides. During the synthesis of an anti-cancer molecule, Azatoxin analogues in an ongoing project in the laboratory it was observed that ortho-halo substituted benzamide analogues of simple amino acid esters showed complex ^{1}H and ^{13}C NMR spectra with multiple peaks for single proton. These puzzling results encouraged to investigate further the rotational behaviour of this kind of molecule elaborately. Hence, in this chapter, ortho-halo substituted benzamide derivatives were synthesized and their rotational behaviour was studied. In the course of this study, the influence of an ester functionality on the rotational behaviour of the amide bond in a complex molecule (Azatoxin framework) was revealed. Rotational isomers were not observed when the appended ester functionality was reduced to the corresponding alcohols.

In the next chapter, a palladium-catalyzed C(sp^3)-H arylation followed by de-esterification reactions was reported. A number of isoindolinone and indolinone derivatives were synthesised by the said method. This protocol was further elaborated by synthesising Azatoxin analogues. A probable mechanism of the synthetic scheme was proposed. In the fourth and final chapter inhibition of the liquid-liquid phase separation (LLPS) of alpha-synuclein protein, which is responsible for the fibrillation/aggregation phenomenon by some Zwitter ionic molecules is reported. The pathophysiology of Parkinson's disease (PD) is controlled by an intrinsically disordered protein called alpha-synuclein (α-Syn). The research was focused on synthesizing a small series of pyridine-derived zwitter ionic molecules and studying their efficacies towards modulating the α-Syn aggregation phenomenon via inhibition of LLPS.

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