NED University of Engineering & Technology

Masters Thesis Information Showcase
Spring Semester-2026
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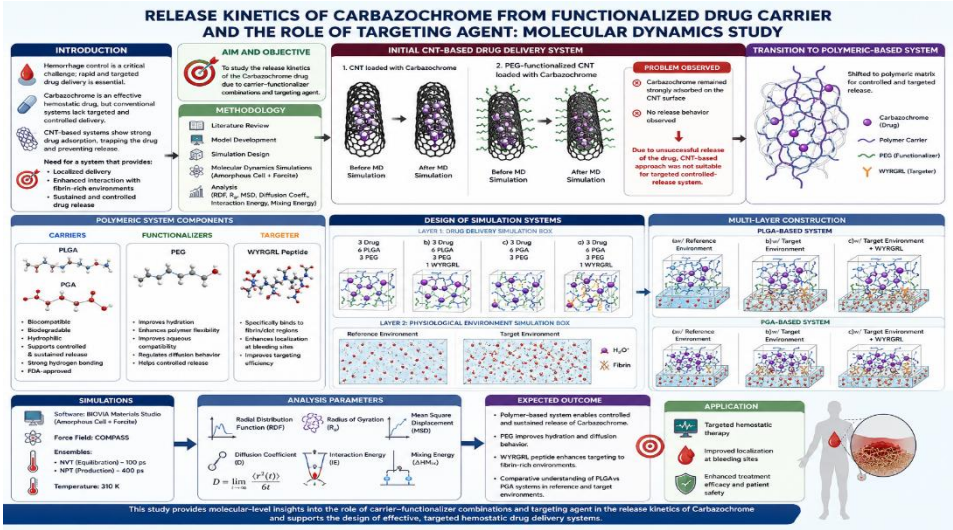
	Department: Biomedical Engineering Programme: Master's in Engineering Specialization: Biomedical Engineering
1	**Title of the Thesis** Release Kinetics of Carbazochrome from Functionalized Drug Carrier and the Role of Targeting Agent: Molecular Dynamics Study
2	**Abstract** (min 300 to 500 words) Hemorrhage remains one of the leading causes of preventable mortality worldwide, making the development of effective hemostatic drug delivery systems an important area of biomedical research. Conventional drug delivery methods often fail to provide controlled and site-specific drug release, resulting in reduced therapeutic efficiency and potential systemic side effects. Carbazochrome is a widely used hemostatic agent; however, its clinical performance can be enhanced through an optimized delivery system capable of releasing the drug in a controlled manner at bleeding sites. The objective of this study was to investigate the release kinetics of Carbazochrome using different carrier–functionalizer combinations and to evaluate the role of a targeting agent through molecular dynamics simulations. The study initially explored a carbon nanotube (CNT)-based drug delivery system, both with and without polyethylene glycol (PEG) functionalization. Simulation results demonstrated that Carbazochrome remained strongly adsorbed on the CNT surface, preventing effective drug release. Due to this limitation, the CNT-based approach was considered unsuitable for achieving controlled and targeted drug delivery. Consequently, the research shifted to biodegradable polymeric carriers, namely poly(lactic-co-glycolic acid) (PLGA) and poly(glycolic acid) (PGA), functionalized with PEG to improve hydration, compatibility, and diffusion characteristics. The fibrin-targeting peptide WYRGRL was further incorporated to enhance localization of the drug delivery system at bleeding sites. A series of molecular dynamics simulations were performed using BIOVIA Materials Studio, employing the COMPASS force field under NVT and NPT ensembles. The formulations were evaluated using mean square displacement (MSD), diffusion coefficient, interaction energy, and other molecular analyses to understand the release behavior of Carbazochrome. Comparative analysis revealed that the PGA-based formulation containing PEG and WYRGRL (Combination 3) exhibited the strongest molecular interactions, the lowest diffusion coefficient, and the most sustained and controlled drug release among all tested systems. In contrast, the PLGA formulations showed inconsistent release behavior, while the CNT-based system failed to release the drug effectively. Overall, the findings demonstrate that the PGA–PEG–WYRGRL formulation is the most promising candidate for targeted hemostatic drug delivery. This study provides valuable molecular-level insights into the design of biodegradable polymeric drug carriers and highlights the importance of carrier selection, functionalization, and targeting strategies in developing efficient controlled-release systems for hemorrhage management.

3	**Impact on SDG#___"** (min 500 words) **SDG 3 – Good Health and Well-being:** This research directly contributes to United Nations Sustainable Development Goal **(SDG) 3: Good Health and Well-Being** by supporting the development of safer and more effective drug delivery technologies for hemorrhage management. Excessive bleeding is a major cause of mortality in trauma, surgery, and emergency medical conditions, emphasizing the need for innovative therapeutic approaches that improve treatment outcomes while minimizing adverse effects. The proposed polymeric drug delivery system was designed to enhance the controlled and localized release of Carbazochrome, allowing the drug to be delivered more efficiently to fibrin-rich bleeding sites. The molecular-level understanding generated through this research provides a scientific foundation for future hemostatic drug delivery systems and contributes to innovations that can strengthen healthcare outcomes, improve the quality of emergency treatment, and ultimately support healthier lives and well-being for patients worldwide.
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6	**Graphical Abstract**