

RESEARCH ARTICLE

In Silico Investigation of Luminol, Its Analogues and Mechanism of Chemiluminescence for Blood Identification Beyond Forensics

Toluwase H. Fatoki^{1,2,*}

¹Translational Bioinformatics Unit, Department of Biochemistry, Federal University Oye-Ekiti, PMB 373, Oye-Ekiti, Ekiti State, Nigeria; ²Fhezt Bioinformatics Laboratory, Ifaki-Ekiti, Ekiti State, Nigeria

Abstract: Objective: This study aimed at discovering chemiluminescent analogues of luminol, predict their molecular binding to hemoglobin of bloodstains in household crime, and expound the mechanism of chemiluminescence of luminol.

Methodology: Similarity and clustering analyses of luminol analogues were conducted, and molecular docking was carried out using hemoglobin from *Homo sapiens* and four domestic organisms namely *Gallus gallus*, *Drosophila melanogaster*, *Rattus norvegicus*, and *Canis familiaris*.

Results: The results showed the order of overall binding score as *D. melanogaster* > *H. sapiens* > *C. familiaris* > *R. norvegicus* > *G. gallus*. Seven compounds namely ZINC16958228, ZINC17023010, ZINC19915427, ZINC34928954, ZINC19915369, ZINC19915444, and ZINC82294978, were found to be consistently stable in binding with diverse hemoglobin and possibly have chemiluminescence than luminol in this *in silico* study. The interaction of human hemoglobin with luminol and its analogues, showed that amino acid residues His45, Lys61, Asn68, Val73, Met76, Pro77, Ala79, Ala82, Leu83, Pro95, Phe98, Lys99, Ser102, Ser133, Ala134, and Thr134, were possibly significant in the mechanism of action of presumptive test compounds. It was hypothesized that the improved mechanism of chemiluminescent for the identification of blood was based on peroxidase-like reaction, that produces nitric oxide which binds to hemoglobin (Hb) and inhibits Hb degradation without yielding fluorescent products. The compound 2,3-benzodioxine-1,4,5(6H)-trione was formed, which possibly emits light.

Conclusion: This study provides novel insight on the luminol and its expanded mechanism for broader possible applications with careful development of new methodologies.

Keywords: Luminol, chemical analogues, molecular docking, hemoglobin, chemiluminescence, mechanism design.

1. INTRODUCTION

Forensic biology is an aspect of forensic science that comprises of serology and deoxyribonucleic acid (DNA) analyses. In the forensic investigation laboratory, serological analysis deals with the screening of evidence for the presence of body

fluids (such as bloodstains, saliva and semen) while DNA profiling is used to pinpoint body fluids to a specific organism. However, the strengths and present limitations of DNA profiling have been presented [1]. Blood is an important body fluid that is required for living systemic activities, which consist of many components (cells, hemoglobin, proteins antibody, clotting factor *etc*), and blood is useful for metabolic profiling in relevance to forensic toxicology and forensic pathology. The identification of blood is central to most crimes

*Address correspondence to this author at the Translational Bioinformatics Unit, Department of Biochemistry, Federal University Oye-Ekiti, PMB 373, Oye-Ekiti, Ekiti State, Nigeria; E-mail: toluwase.fatoki@fuoye.edu.ng, fheztbioinformatics@gmail.com