**MOLECULAR DOCKING STUDIES OF ARYLSUBSTITUTED IMIDAZOLES AND THE ONCOGENIC PROTEIN *BCR-ABL* *TYROSINE KINASE*.**

**MSc. Julio A. Rojas Vargas**1, PhD América García López1, Est. Lianne Álvarez Rodríguez1, Prof. PhD Matheus Froeyen2

1Chemistry Department, Exact and Natural Science Faculty, Oriente University, Santiago de Cuba, Cuba, [jarojas@uo.edu.cu](mailto:jarojas@uo.edu.cu) [america@uo.edu.cu](mailto:america@uo.edu.cu)

2Medicinal Chemistry, Department of Pharmacy, Rega Institute, KU Leuven, Leuven, Belgium.

[mathy.froeyen@kuleuven.be](mailto:mathy.froeyen@kuleuven.be)

**Abtract**

The treatment of chronic myeloid leukemia (CML) should be considered one of the medical successes of the last 30 years. CML is a myeloproliferative disorder that seriously compromises the health and lifestyle of the patient who suffers. If not detected in time, the evolution of it can lead to a fatal end. The Philadelphia Chromosome (CrPh) is present in approximately 95% of patients with CML, constituting a diagnostic marker of the disease. It is formed by the Bcr-Abl oncogene. In the present work it was carried out a molecular docking study between 12 arylsubstituted imidazoles and two oncogene protein Bcr-Abl, Abl kinase (3CS9) and T315I mutation (2V7A). To carry out the molecular docking, the Autodock 4.2 program was used, while the crystalline structures of the proteins were extracted from the Protein Data Bank database. A docking study was also carried out with co-crystalized substrates in each protein and a set of drugs currently used against CML. According to the results obtained, imidazoles 5a, 5d and 5j have a greater affinity towards the Abl kinase, whereas 5e, 5g and 5i towards the T315I mutation. In addition, these imidazoles were found to have better couplings than the substrates and drugs studied, only surpassed by Dasatinib and Ponatinib.

**Keyword.**

Chronic Myeloid Leukemia (CML), Molecular docking, aryl-substituted imidazoles, protein Bcr-Abl.