10th Brazilian Conference on Natural Products
XXXVI RESEM
4-7 November 2025, Belo Horizonte, MG, Brazil

Section: 03

IN SILICO STUDY OF SILYMARIN COMPOUNDS AGAINST Helicobacter pylori VIRULENCE FACTORS

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Helicobacter pylori is a bacteria capable of colonizing the human stomach, which makes it the greatest risk factor for stomach cancer development. The drugs used in its treatment, like clarithromycin, have already shown resistance, showing the need for the development of new drugs against this infection. Silymarin, which is a complex of flavonolignans extracted from the plant *Silybum marianum* (L.) Gaertn., is traditionally and safely used to treat liver diseases and has already shown anti-*H. pylori* activity in previous *in vitro* assays. This study aimed to evaluate the potential of the main silymarin compounds (silybinin A and B, isosilybinin A and B, silychristin, isosilycrhristin, taxifolin and silydianin) of inhibiting virulence factors of *H. pylori* and their drug-likeness properties through *in silico* techniques. The platforms SwissADME and ADMETlab 3.0 servers were used to analyse the physicochemical, pharmacokinetics and druglikeness profile. The results demonstrated that the compounds exhibit values for LogP ranging from 0,85 to 1,85, LogS ranging from -4,45 to -3,33. All compounds were approved in the Lipinski rule. The molecular docking was executed with GOLD software with the protein targets BabA (PDB: 4ZH7), CagA (PDB: 4IRV) and VacA (PDB: 2QV3), and it was detected that most of the compounds are able to establish interactions the essential aminoacids CYS189, GLY191 and SER244 of BabA (with the best fitness score 57,7528 for isosilybinin A), with the essential aminoacids VAL107, PHE219 and TRP212 of CagA (with the best fitness score 63,0801 for silychristin), and with the aminoacids VAL266 and ASN289 of VacA (with the best fitness score 54,5783 for isosilybinin B). Therefore, it is possible to conclude that the silymarin compounds possess good drug-likeness profile and are capable to establish positive molecular interactions with the tested proteins, and therefore, are suitable enter experimental essays with the possibility of representing a new frontier against *H. pylori* and the consequential reduction of the risk of stomach cancer development in the future. The authors thank the support from UFES and FAPES.

Keywords: *Helicobacter pylori; virulence factors; natural compounds, silymarin; in-silico techniques.*