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IN SILICO EVALUATION OF FLAVONOIDS FOR INHIBITION OF THE ENZYMES GLUCOSE 6-PHOSPHATE DEHYDROGENASE, SHIKIMATE KINASE AND ASPARTATE SEMIALDEHYDE DEHYDROGENASE ENZYMES OF Helicobacter pylori

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Helicobacter pylori is a microaerophilic, Gram-negative bacterium that colonizes the human gastric mucosa and constitutes the main risk factor for gastric adenocarcinoma. Increasing bacterial resistance and adverse effects of conventional treatment encourage the search for therapeutic alternatives, including natural compounds with antimicrobial potential. This study aimed to perform an *in silico* evaluation of flavonoids described in the literature as having anti-*H. pylori* activity and evaluate their ability to inhibit three target enzymes of bacterial metabolism: glucose-6-phosphate dehydrogenase (HpG6PD), shikimate kinase (SK), and aspartate semialdehyde dehydrogenase (ASADH). The flavonoids were selected from a literature review using the PubMed and SciELO database. Their physicochemical and pharmacokinetic properties were predicted by SwissADME server. Subsequently, molecular docking assays were performed on SwissDock/AutoDock Vina, with pose analysis in Discovery Studio. Forty flavonoids with anti-*H. pylori* activity were identified, of which 23 presented adequate pharmacokinetic properties: partition coefficient ranging from 3.76 to 0.51, high gastrointestinal absorption, non-permeability in the blood-brain barrier and compliance with Lipinski's rule. Docking indicated relevant interactions with the three enzymes. For SK, morin (-7,122 kcal/mol), diosmetin (-6,377 kcal/mol) and taxifolin (-6,533 kcal/mol) presented the best interaction. For ASADH and HpG6PD, licoisoflavone B presented the highest layers (-8,150 and -8,695 kcal/mol, respectively), followed by luteone (-7,467 and -8,255 kcal/mol) and isowigtheone (-7,256 and -8,039 kcal/mol). These results highlighted a potential against *H. pylori* infection and its complications. Flavonoids such as licoisoflavone B, luteone, isowigtheone, and morin have a promising profile against the essential enzymes of *H. pylori*. These results reinforce the need for *in vitro* experimental validation to confirm their therapeutic applicability.

Keywords: *Helicobacter pylori. Stomach cancer. Flavonoids.*

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