TITLE: SCREENING OF PLANT COMPOUNDS WITH ANTI-QUORUM SENSING POTENTIAL BY MOLECULAR DOCKING WITH SdiA PROTEIN FROM *Salmonella* Enteritidis

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ABSTRACT:
Salmonella strains are frequently involved in foodborne diseases. Biofilm production and expression of virulence genes in this pathogen are regulated by a communication mechanism called quorum sensing (QS). *Salmonella* does not produce the QS signaling molecule acyl homoserine lactone (AHL), but it uses the SdiA protein, a LuxR homolog, to respond to AHLs produced by other bacteria. Some studies have suggested that plant phenolic compounds can act inhibiting QS regulated phenotypes. Therefore, the purpose of this work was to evaluate and compare the binding of methoxy phenolics compounds such as shogaol, isoshogaol and gingerol with different carbon size chains as well as AHLs and furanones to the *Salmonella* Enteritidis SdiA protein by molecular docking. The CLC Drug Discovery Workbench 3.0.2 software and the structure of *Escherichia coli* enterohemorrhagic (EHEC) SdiA protein available in the Protein Data Bank (PDB: 4Y13) were used to model the SdiA protein of *Salmonella enterica* serovar Enteritidis PT4 578 (GenBank: AGZ95694.1) which has not yet been crystallized. The molecular docking of this protein was performed with methoxy phenolic compounds, AHLs and furanones using the above mentioned software. Among the analyzed compounds, [6]-shogaol was the one with the best linkage score (-67.94) to SdiA protein of *Salmonella* Enteritidis, which was as high as that of the N-(3-oxododecanoyl)-L-homoserine lactone a molecule shown to bind to SdiA *in vivo* and *in vitro* in previous studies. The other compounds as well as their binding scores were [8]-shogaol (-64.77), [6]-isoshogaol (-61.81) and [6]-gingerol (-61.34). All these compounds presented better binding scores than furanones which have are known QS inhibitors. The results indicate that phenolic compounds possibly are able to bind SdiA protein of *Salmonella* confirming their potential as quorum sensing inhibitors.

Keywords: inhibitors, methoxy phenol, pathogen, quorum sensing, quorum quenching.

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