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Identification of small molecule inhibitors against SecA of *Candidatus Liberibacter asiaticus* by structure based design

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Huanglongbing is the most devastating disease of citrus caused by *Candidatus Liberibacter asiaticus* (Las) (1, 2). In the present study, we report the discovery of novel small molecule inhibitors against SecA ATPase of Las by using structure based design methods. We built the homology model of SecA protein structure of Las based on the SecA of *Escherichia coli*. The model was used for *in-silico* screening of commercially available compounds from ZINC database. Using the glide flexible molecular docking method, twenty structures were chosen for *in vitro* studies. Five compounds were found to inhibit the ATPase activity of SecA of Las at nano molar concentrations and showed antimicrobial activities against *Agrobacterium tumefaciens* with MBC ranging from 128 to 256

□g/mL. These as lead compounds for further development of antimicrobial compounds against Las. To test the application potential of those compounds on plants, the phytotoxicity studies were performed on the five compounds against citrus. In addition, we are optimizing these five antimicrobial compounds to identify compounds higher antimicrobial activity.

References

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