

# UC Riverside

## Journal of Citrus Pathology

### Title

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

### Permalink

<https://escholarship.org/uc/item/9k6712tj>

### Journal

Journal of Citrus Pathology, 1(1)

### Authors

Akula, Nagaraju  
Trivedi, Pankaj  
Han, Frank Q.  
et al.

### Publication Date

2014

### DOI

10.5070/C411025216

### Copyright Information

Copyright 2014 by the author(s). This work is made available under the terms of a Creative Commons Attribution License, available at <https://creativecommons.org/licenses/by/4.0/>

## 9.11 P

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

Akula, N.<sup>1</sup>, Trivedi, P.<sup>1</sup>, Han, F.Q.<sup>2</sup>, and Wang, N.<sup>1,\*</sup>

<sup>1</sup>Citrus Research & Education Center, Department of Microbiology and Cell Science, University of Florida, 700 Experiment Station Rd., Lake Alfred, FL 33850, USA

<sup>2</sup>Structure Based Design, Inc., 6048 Cornerstone Court West, Suite D, San Diego, CA 92121, USA

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

Bové, JM. Huanglongbing: A destructive, newly-emerging, century-old disease of citrus. 2006. Journal of Plant Pathology, 88 (1), 7-37.

Gottwald, TR, da Graça, JV, and Bassanezi, RB. 2007. Citrus Huanglongbing: The pathogen and its impact. Online. Plant Health Progress doi:10.1094/PHP-2007-0906-01-RV.