

FLORIDA STATE UNIVERSITY  
COLLEGE OF ARTS AND SCIENCES

PROTEIN LIGAND BINDING MOLECULAR DYNAMICS SIMULATIONS  
AND LARGE-SCALE LEAD IDENTIFICATION

By

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A Dissertation submitted to the  
Department of Chemistry and Biochemistry  
in partial fulfillment of the  
requirements for the degree of  
Doctor of Philosophy

2024

Zilin Huang defended this dissertation on March 26, 2024.

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