

# RESEARCH ARTICLE

## Molecular determinants of orthosteric–allosteric dual inhibition of PfHT1 by computational assessment

Decheng Kong<sup>1,\*</sup>, Jinlong Ren<sup>1,\*</sup>, Zhuang Li<sup>1</sup>, Guangcun Shan<sup>2,3,5,6,†</sup>, Zhongjian Wang<sup>2</sup>,

Ruiqin Zhang<sup>3</sup>, Wei Huang<sup>5</sup>, Kunpeng Dou<sup>1,4,‡</sup>

<sup>1</sup>College of Physics and Optoelectronic Engineering, Faculty of Information Science and Engineering, Ocean University of China, Qingdao 266100, China

<sup>2</sup>BCPMdata Pharma Technology (Chengdu) Co. Ltd, Chengdu 610095, China

<sup>3</sup>Department of Physics, City University of Hong Kong, Hong Kong SAR 999077, China

<sup>4</sup>Engineering Research Center of Advanced Marine Physical Instruments and Equipment of Education Ministry of China & Key Laboratory of Optics and Optoelectronics of Qingdao, Ocean University of China, Qingdao 266100, China

<sup>5</sup>School of Flexible Electronics, Sun Yat-sen University, Shenzhen 518107, China

<sup>6</sup>Institute of Precision Instrument and Quantum Sensing & Beijing Advanced Innovation Center for Big Data-based Precision Medicine, Beihang University, Beijing 100191, China

\*These authors contributed equally to this work.

Corresponding authors. E-mail: <sup>†</sup>gshan2-c@my.cityu.edu.hk, <sup>‡</sup>doukunpeng@ouc.edu.cn

Received April 10, 2025; accepted May 6, 2025

### Supporting Information

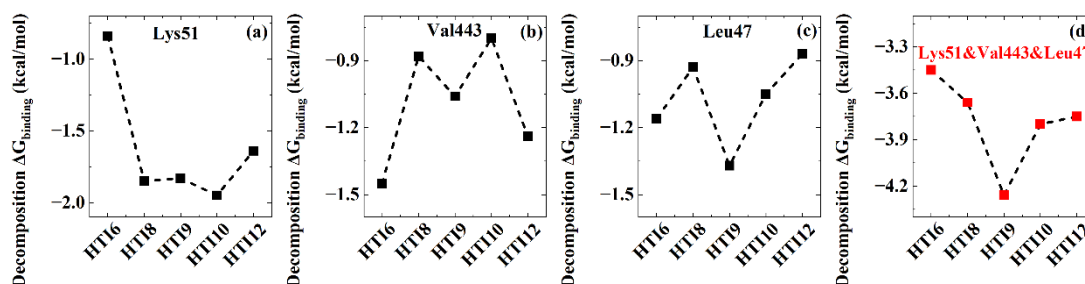


Fig. S1 Decomposed contribution of key residues to  $\Delta G_{\text{binding}}$  for group I.

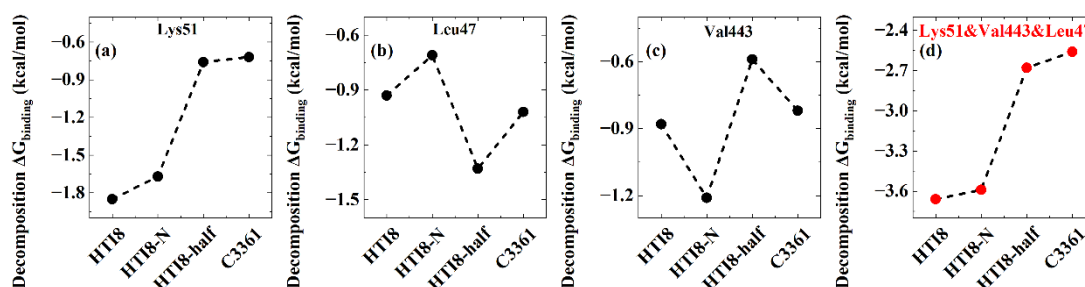


Fig. S2 Decomposed contribution of key residues to  $\Delta G_{\text{binding}}$  for group II.