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Identification of small-molecule binding sites of a ubiquitin-conjugating enzyme-UBE2T through fragment-based screening

Protein Science
15 February 2024


Yong Yao Loh, Jothi Anantharajan, Qiwei Huang, Weijun Xu, Justina Fulwood, Hui Qi Ng, Elizabeth Yihui Ng, Chong Yu Gea, Meng Ling Choong, Qian Wen Tan, Xiaoying Koh, Wan Hsin Lim, Kassoum Nacro, Joseph Cherian, Nithya Baburajendran, Zhiyuan Ke, CongBao Kang



A high-throughput cell-based screening method for Zika virus protease inhibitor discovery.

SLAS
23 May 2024


Paulina Duhita Anindita, Yuka Otsuka, Simon Lattmann, Khac Huy Ngo, Chong Wai Liew, CongBao Kang, Reuben S. Harrise, Louis Scampavia, Timothy P. Spicer, Dahai Luo



Ultra-large scale virtual screening identifies a small molecule inhibitor of the Wnt transporter Wntless

iScience
04 July 2024

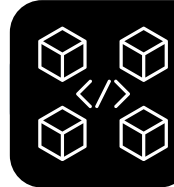
Jia Yu, Pei-Ju Liao, Thomas H. Keller, Joseph Cherian, David M. Virshup, Weijun Xu



Pharmacodynamic evaluation of AUM001/tinodasertib, an oral inhibitor of mitogen-activated protein kinase (MAPK)-interacting protein kinase 1, 2 (MNK1/2) in preclinical models and tissues from a Phase 1 clinical study.

Journal of Cancer Science and Clinical Therapeutics
16 August 2024


Bong Hwa Gan, Lay Hoon Lee, Reika Takeda, Maryam Yasin, Vincenzo Teneggi, Kantharaj Ethirajulu, Pauline Yeo, Dhananjay Umrani, Vishal Pendharkar, Darren Wan Teck Lim, Greg Li, Qingshu Lu, Yang Cao, Ranjani Nellore, Stephanie Blanchard, Hannes Hentze, Veronica Novotny-Diermayr



Protocol to perform fragment screening using NMR spectroscopy.

STAR Protocols
22 August 2024

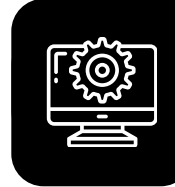
Qiwei Huang, CongBao Kang



Regio-MPNN: predicting regioselectivity for general metal-catalyzed cross-coupling reactions using a chemical knowledge informed message passing neural network

Digital Discovery
03 September 2024


Baochen Li, Yuru Liu, Haibin Sun, Rentao Zhang, Yongli Xie, Klement Foo, Frankie S. Mak, Ruimao Zhang, Tianshu Yu, Sen Lin, Peng Wang and Xiaoxue Wang



Current Status of Computational Approaches for Small Molecule Drug Discovery.

Journal of Medicinal Chemistry
24 October 2024

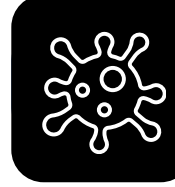
Weijun Xu



Button-Push On-Demand Synthesis for Rapid Optimization of Antiviral Peptidomimetics

Journal of the American Chemical Society
30 October 2024

Duanshuai Tian, Ting Wei Tan, Ronald Toh Kuan Hai, Gan Wang, Fadhil Peer Mohamed, Zhenyang Yu, Hwee Ting Ang, Weijun Xu, Qian Wen Tan, Pearly Shuyi Ng, Choon Heng Low, Boping Liu, Perlyn Quek Zekui, Joma Kanikadu Joy, Joseph Cherian, Frankie S Mak, Jie Wu



^1H , ^{15}N and ^{13}C backbone resonance assignment of the N-terminal region of Zika virus NS4B protein in detergent micelles

Biomolecular NMR Assignments
07 November 2024

Yan Li, Ying Ru Loh, Qingxin Li, Dahai Luo, CongBao Kang