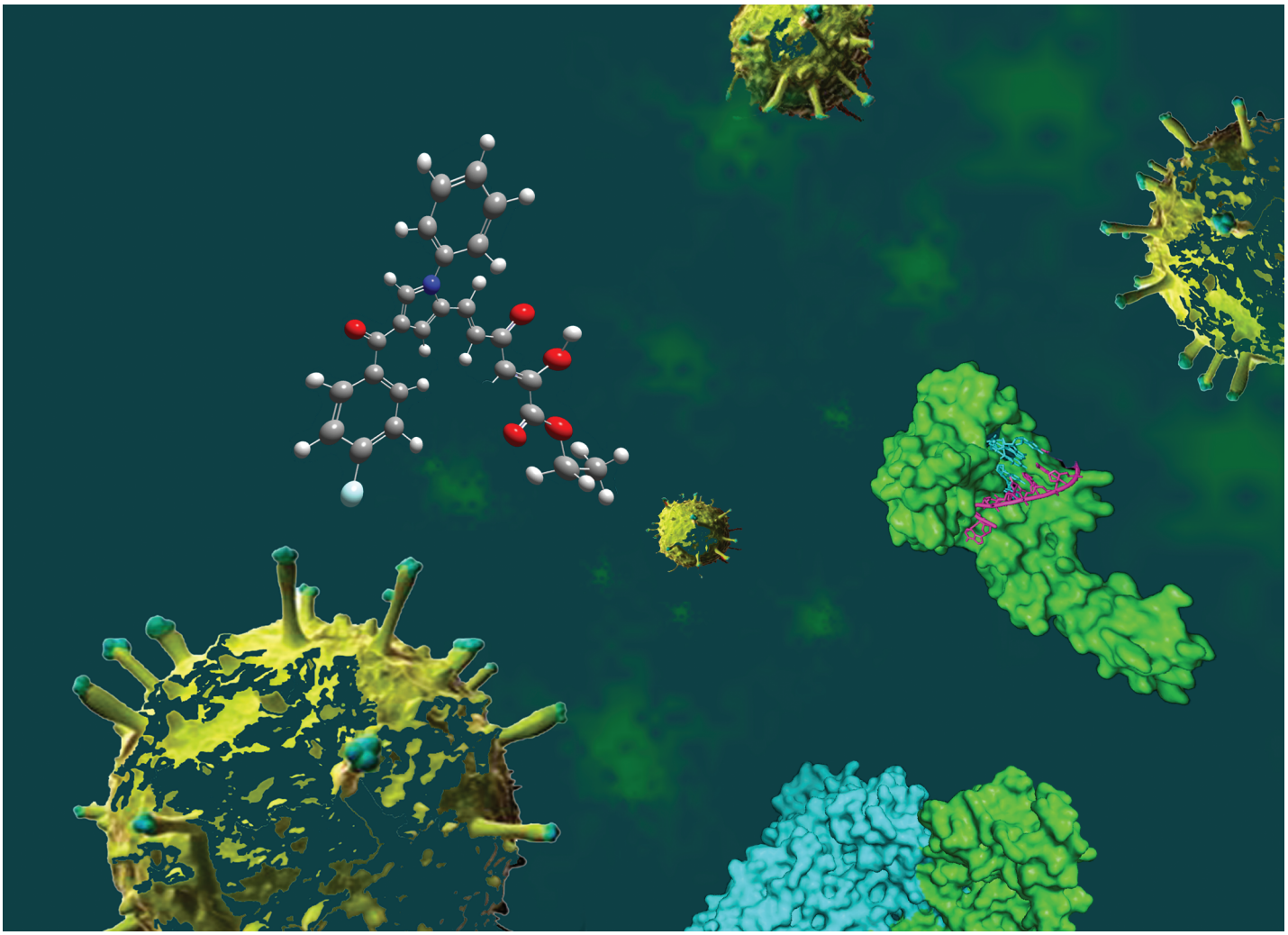

Showcasing research from the Group of Assoc. Prof. Weiwei Xue and Prof. Feng Zhu at Chongqing University and Zhejiang University, China

Prediction of the binding mode and resistance profile for a dual-target pyrrolyl diketo acid scaffold against HIV-1 integrase and reverse-transcriptase-associated ribonuclease H

The Innovative Drug Research and Bioinformatics (IDRB) group is working on the binding mechanism identification and structure-based design of multi-target drugs for complex diseases, such as mood disorders and HIV infection. Multi-target drugs have the benefits of rapid onset and/or higher efficacy for complex disease treatment. This computational work predicts the binding mode and potential resistance profile of the dual-target pyrrolyl diketo acid scaffold against HIV-1 integrase (IN) and the reverse-transcriptase-associated ribonuclease H (RNase H) active sites.

As featured in:

See Weiwei Xue, Feng Zhu *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 23873.

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