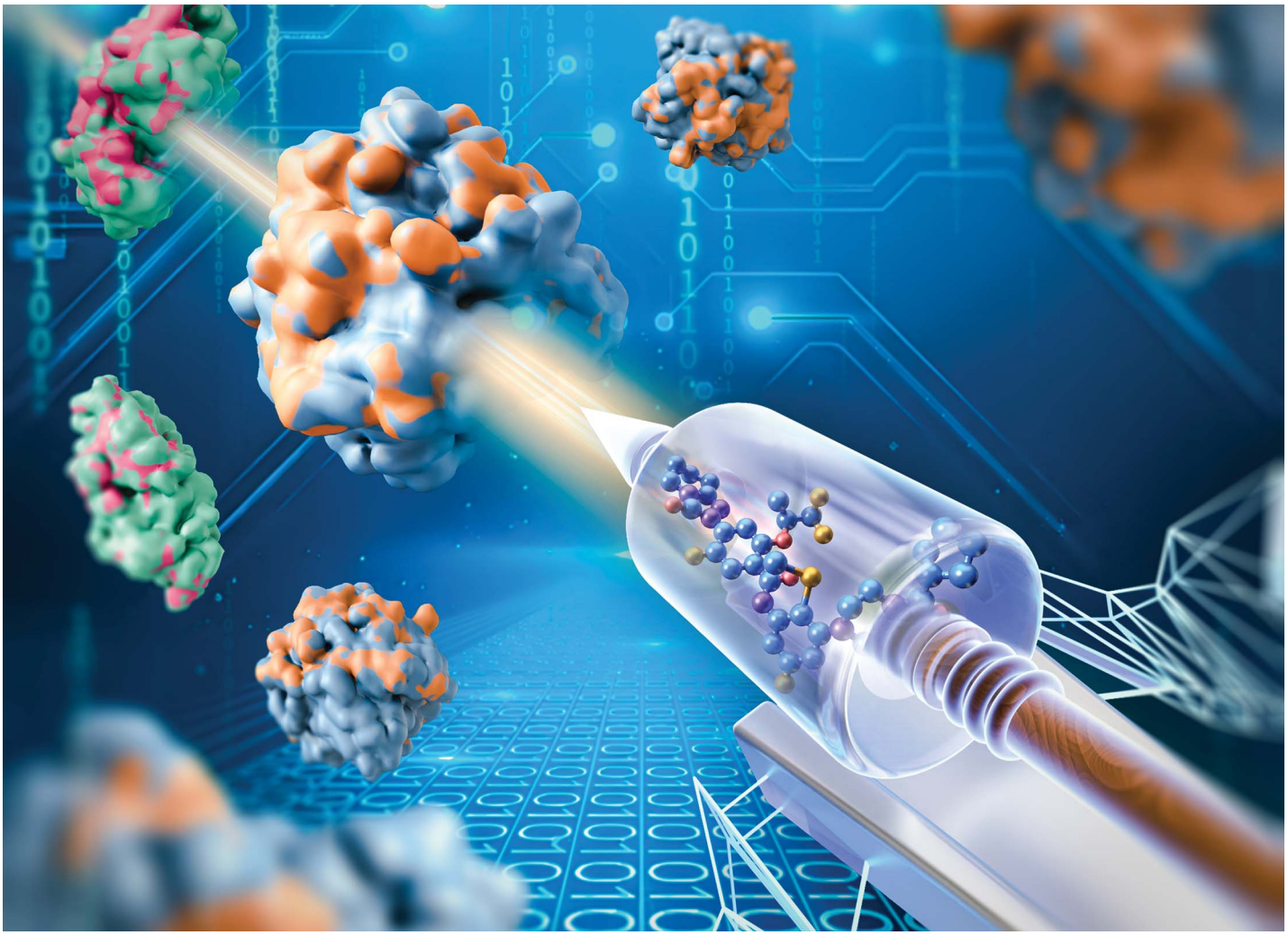

Showcasing research from Professor Yuedong Yang's laboratory, School of Computer Science and Engineering, Sun Yat-sen University, Guangzhou, China.

Structure-aware dual-target drug design through collaborative learning of pharmacophore combination and molecular simulation

Given the challenges often faced by single-target drugs like drug resistance, the design of dual/multi-target drugs has gained considerable attention as an appealing strategy. This study introduces AIxFuse, an innovative dual-target drug design method that integrates pharmacophore combination and molecular simulation through reinforcement learning and active learning techniques. AIxFuse demonstrates a significantly higher success rate compared to existing technologies and showcases its ability to generate compounds with improved dual-target binding affinities and structural interpretability. This methodology holds great promise for expediting the development of anti-resistance drugs for complex diseases.

As featured in:

See Yuedong Yang *et al.*, *Chem. Sci.*, 2024, **15**, 10366.

ROYAL SOCIETY OF CHEMISTRY

rsc.li/chemical-science

Registered charity number: 207890