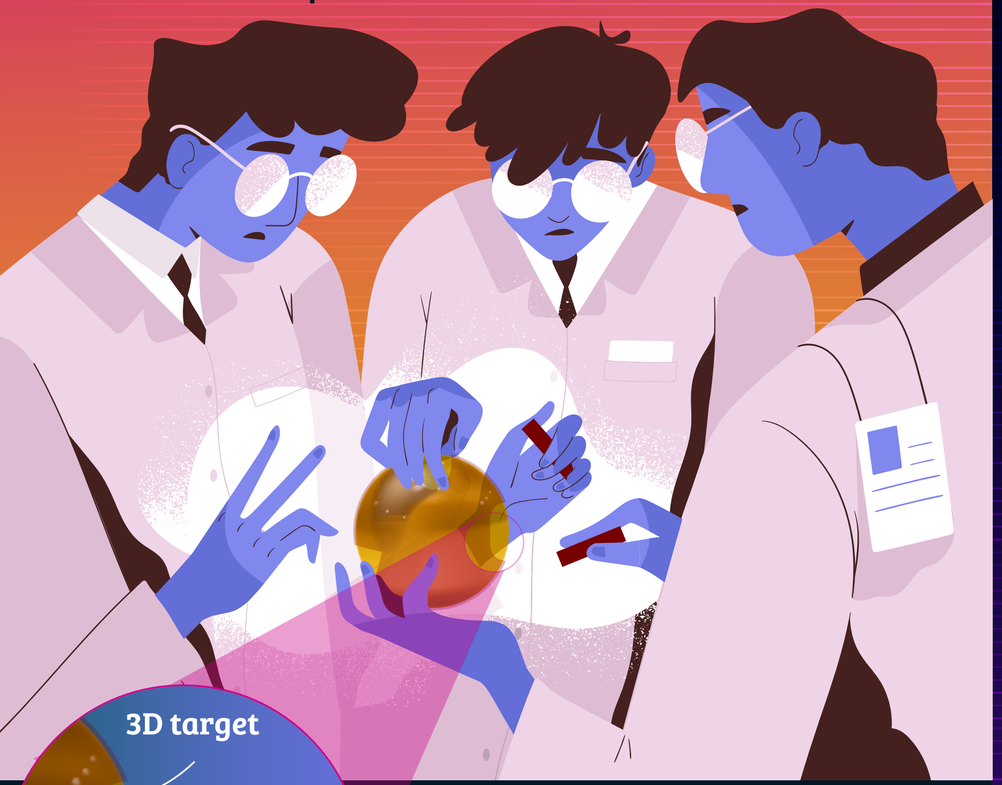
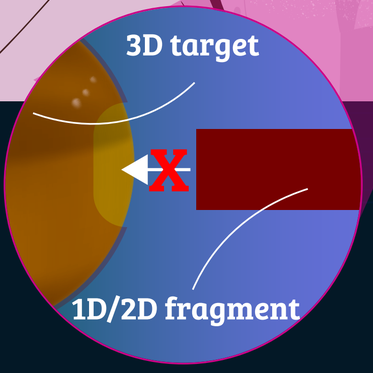
Metallofragments as 3D Scaffolds for Fragment-Based Drug Discovery

Fragment-based drug discovery (FBDD) is a successful strategy for the discovery of small molecule therapeutics

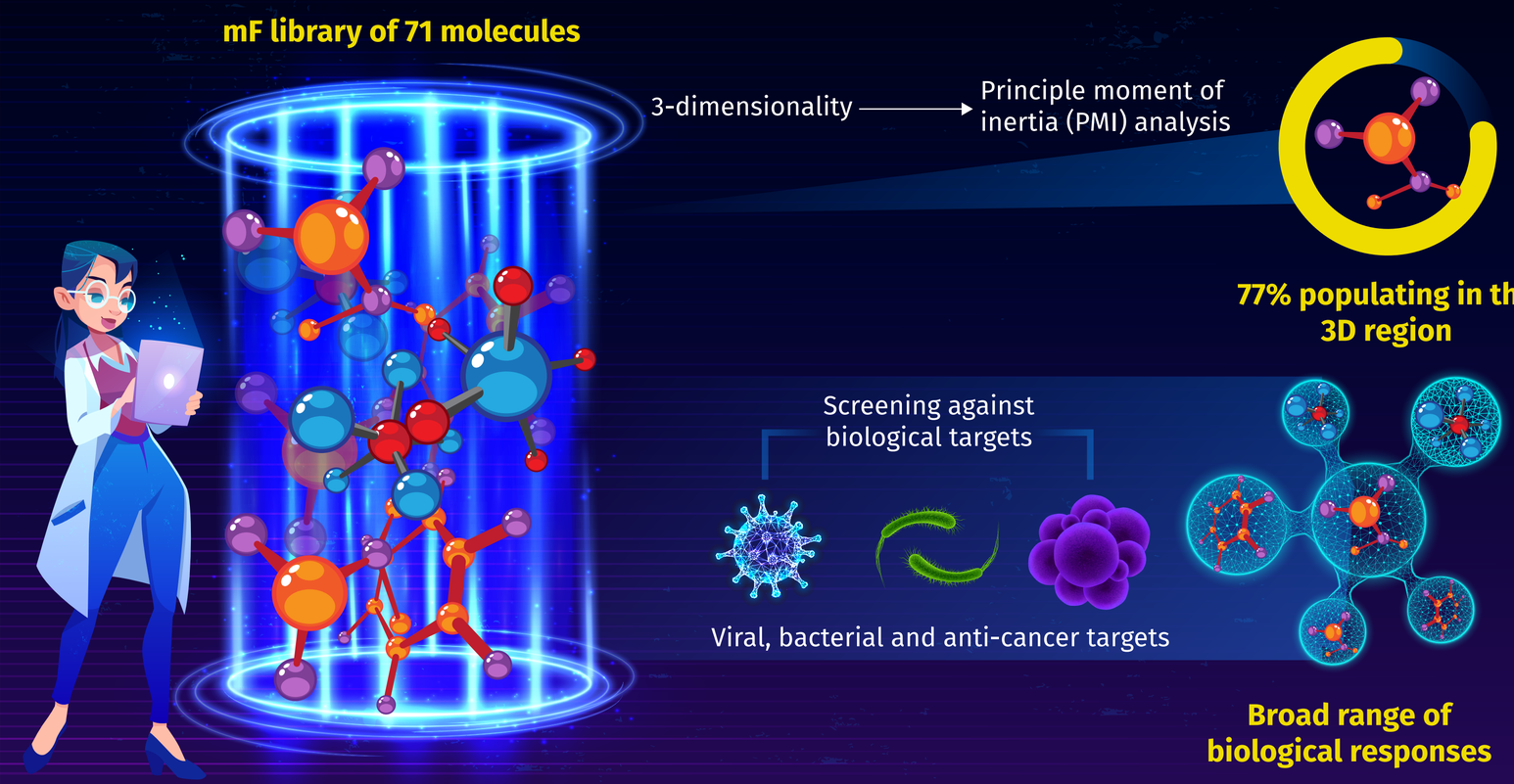




However, the linear (1D) or planar (2D) shape of organic fragments limits a more complete exploration of chemical shape for target protein binding

Inert metal complexes or metallofragments (mFs) can be used to construct 3D fragment libraries

An mF library with 13 classes of metal complexes was designed, synthesized, and characterized



mF libraries access underutilized 3D fragment space for FBDD against a variety of protein targets, which could lead to new opportunities in drug discovery

Chemical Science

PICK OF THE WEEK

Expanding Medicinal Chemistry into 3D Space: Metallofragments as 3D Scaffolds for Fragment-Based Drug Discovery

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