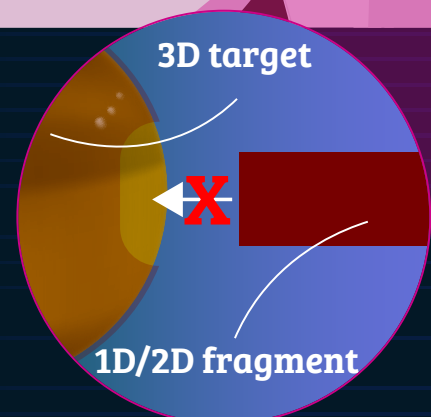


Metallofragments as 3D Scaffolds for Fragment-Based Drug Discovery

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

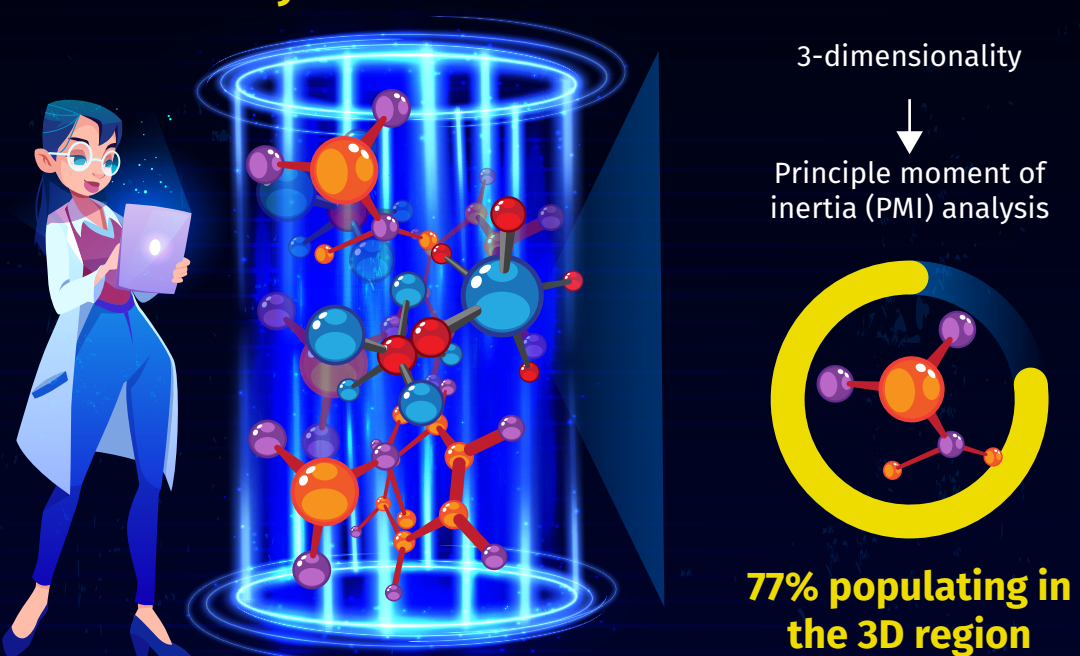


However, the linear (1D) or planar (2D) shape of organic fragments limits a more complete exploration of chemical shape for target protein binding

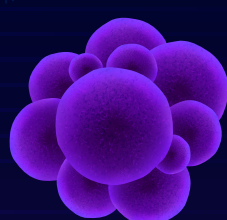
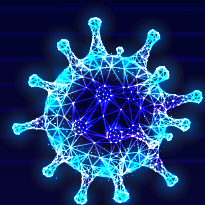
Inert metal complexes or metallofragments (mFs) can be used to construct 3D fragment libraries

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

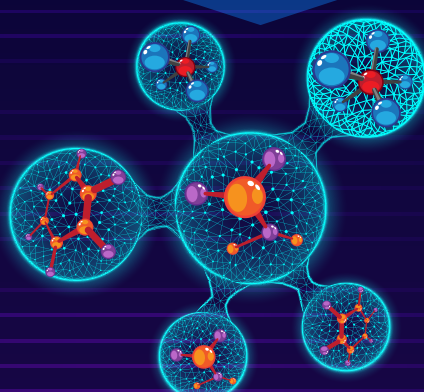
mF library of 71 molecules



Screening against biological targets



Viral, bacterial and anti-cancer targets



Broad range of biological responses

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