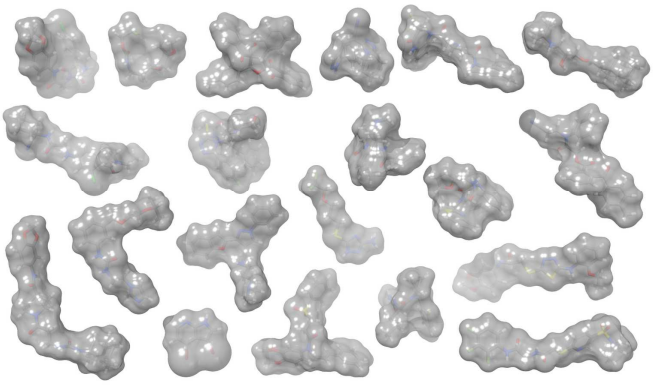
3D DIVERSITY SET

New cost-effective preplated set of screening compounds from Enamine

Specification	
Number of compounds	50,000
Source	Enamine HTS collection (1.2 million compounds)
Novelty	no overlap with previous sets by Enamine
Support services	re-supply in dry powders warranted, re-synthesis, synthesis of focused libraries of analogues, hit-to-lead projects
Purity	at least 90% by LCMS and ^{1}H NMR
Cherry picking	allowed by plates
Formatting options	A. 10 mM solutions in DMSO in 384 well plates (Matrix Cat. No 4312) with columns 1, 2, 23, and 24 empty (filled with pure DMSO). Amounts: 25, 50 and 100 µL
	B. 10 mM solutions in DMSO in 96 well plates (Matrix Cat. No 4919) with columns 1 and 12 empty (filled with pure DMSO). Amounts: Amounts: 50, 100, and 200 µL
	C. 1 mg in 0.75 mL microtubes (Matrix Cat. No 4271) with columns 1 and 12 empty
Selection & Design	
Drug-like filters	Lipinski Ro5 & Veber rule, LogS from -6 to 0.5
Medicinal Chemistry filters	proprietary set of over 100 structural filters excluding toxic and non-complex compounds
Design principle	hybrid approach combining structural analysis, analysis of pharmacophores and 3D shapes

Three-dimensional shape is an essential property of molecules determining their principal ability to bind to biological targets. To maximize biological relevance of a compound library, we sought to use this fundamental property in combination with other design approaches.

We have recently developed a computational protocol enabling achievement of maximum diversity of chemical structures, pharmacophore properties and three-dimensional molecular shapes. A set of drug-like compounds (over 1 million molecules) produced from Enamine HTS collection has undergone conformational analysis and 7 million possible molecular conformations were isolated. The resulting set was sequentially taken through three stages of diverse subset generation, namely the *structure*, *pharmacophore*, and *shape* stage, each intended to achieve maximum diversity in certain property. Specific molecular fingerprints were used at each stage to speed up subset generation.



Examples of shapes in the 3D Diversity Set