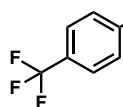


# EnamineREAL

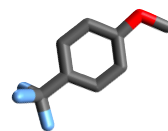


1.4B Molecules

VirtualFlow



SMILES



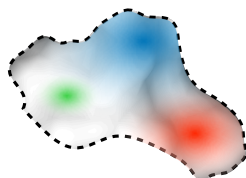
Ready-to-dock  
Conformer

RDKit



Fragment-Protein Complexes

Unsupervised  
Learning



Pharmacophore  
Distribution

FRESCO  
Virtual Screen

Top-500k

Filtering

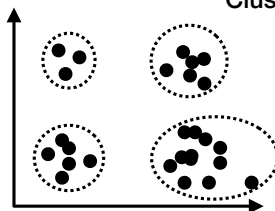
✓ 'lead-like' physchem

✗ PAINS

✓ < 2 chiral centers

Top-50k

Cluster



Top-50

Cluster centroids

