

GT-Predict

3118 reaction classifications  
53 acceptors  
72 enzymes  
11 general + 9 family  
dependent acceptor features

HTS UGT

558 reaction rates  
31 acceptors  
18 enzymes

pTMH

473 reaction rates  
79 acceptors  
6 enzymes

Literature

118 reaction rates  
39 acceptors  
44 enzymes

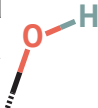
93 reactions  
44 acceptors  
8 enzymes

PubChem

162 SMILES



PubChem  
Conjugate acid  
correction



294 SMILES

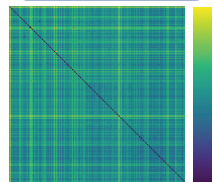


Generate  
negatives

PubChem

Molecular weight  
Charge  
Complexity  
TPSA  
#H-bond donors  
#H-bond acceptors  
#Heavy atoms  
#Rotatable bonds  
#Atom stereos  
#Bond stereos

Pairwise distance

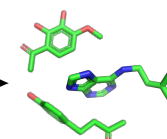


E3FP

Molecular fingerprint

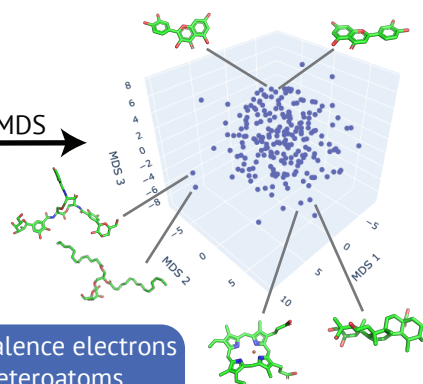


E3FP



SESA

MDS



#Valence electrons  
#Heteroatoms  
#Rings  
#Coumarins  
#Primary alcohols  
...



SASA  
Radius of gyration  
LogP  
...

ProteinVolume



Solvent excluded volume  
Van Der Waals volume  
Void volume  
Packing density