

## GT-Predict

- 3748 reaction classifications
- 72 acceptors
- 72 enzymes
- 11 general + 9 family dependent acceptor features

## Dataset 1

1031 reaction rates  
110 acceptors  
24 enzymes

## Literature

262 reactions  
102 acceptors  
61 enzymes



270 SMILES



PubChem  
Conjugate acid  
correction

2

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

chem

4 P/

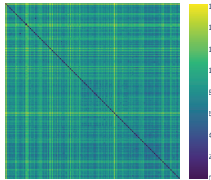
3

3  Generate negatives

## Molecular fingerprint



Pairwise distance



E3FP 9

E3FP



t

70

SESA

MDS

10

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

SASA  
Radius of gyration  
LogP

ProteinVolume 

- Solvent excluded volume
- Van Der Waals volume
- Void volume
- Packing density