

Backend

Promiscuous enzyme dataset



Get Product/SMILES dataset for each promiscuous enzyme

- Filter out common cofactor
- Consider substrate as product for reversible rxns



Get maximal common substructure of products for each promiscuous enzyme



Calculate molecular similarity between maximal common substructure and each product → average out (= maxtoproduct_avg)

Frontend

Input : compound of interest (Pubchem ID)



Check whether there is the maximal common substructure or not in this compound

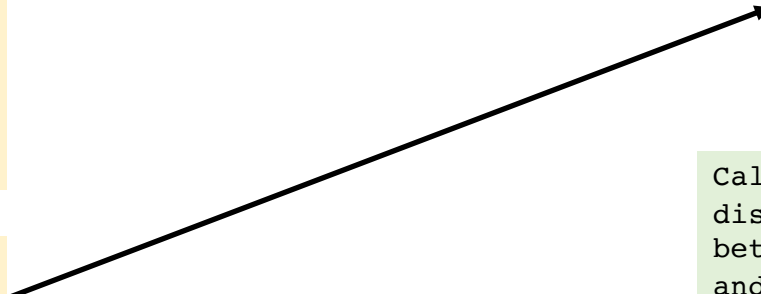
Yes

No

Calculate distance between input and maximal common substructure (maxtoinput)



Rank promiscuous enzyme based on (maxtoinput - maxtoproduct_avg) value



MCSS : maximal common substructure

