Backend

Promiscuous enzyme dataset

↓

Get Product/SMILES dataset for each promiscuous enzyme

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

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Get maximal common substructure of products for each promiscuous enzyme

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

Frontend

Input : compound of interest (Pubchem ID)

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

Yes

Calculate distance between input and maximal common substructure (maxtoinput)

↓

Rank promiscuous enzyme based on (maxtoinput – maxtoproduct_avg) value

No

MCSS : maximal common substructure