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Pattern Analysis between OR and Six Categorized Aromatic Ligands

김명주 (Bioinformatics)

Lab Meeting | August 9, 2024

Agenda

1. Molecular Docking(MD) Program
2. Visualization
3. Random Forest
4. Future Direction

Molecular Docking Program

Chimera X

def)
A next-generation molecular visualization program from the Resource for Biocomputing, Visualization, and Informatics

1. trimming down the PDB file

Open Babel

def)
A chemical toolbox designed to interconvert chemical file formats

1. Converting the Trimmed PDB to a PDBQT File

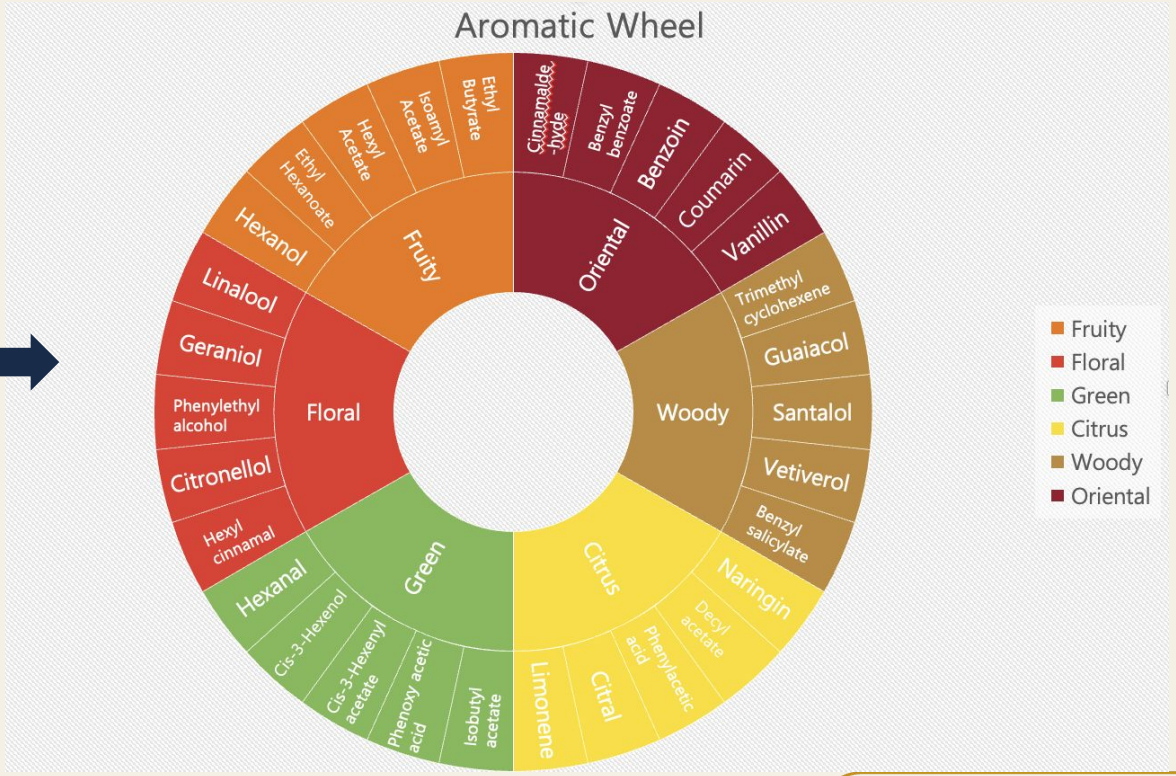
Auto Dock Vina

def)
Molecular Docking(MD) Program

1. taking receptor and ligands in PDBQT format
2. yields binding affinding between receptor and ligand
3. running the automated code, generate the collective result files automatically

Visualization

Six Categorized Aromatic Ligands



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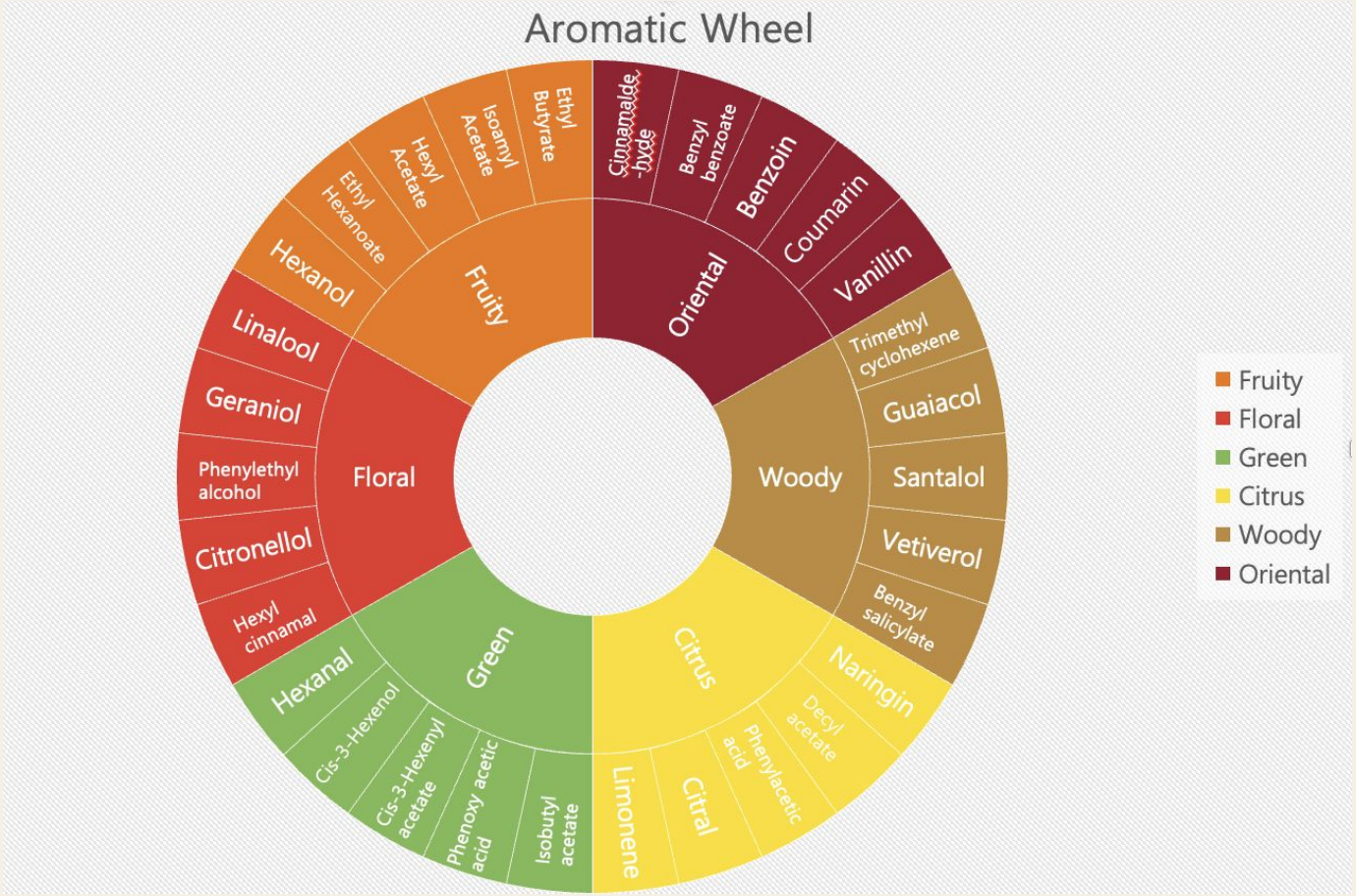
Visualization

1. Citrus
   a. largest affinity range between -4 and -10.
   b. Similar trend ligand binding to ORs, beside Naringin
   c. intuitively similar overall pattern with ‘Green’
2. Floral
   a. intuitively similar overall pattern with ‘Fruity’
   b. in terms of dendrogram of ligand, relates to ‘Green’
3. Woody
   a. intuitively mirrored overall pattern with ‘Oriental’
   b. dendrogram reflects the relationship between ‘Woody' and ‘Oriental’

→ Overall reflects our Aromatic Wheel


Aromatic Wheel
Fruity
Floral
Green
Citrus
Woody
Oriental
Ethyl Butyrate
Isoamyl Acetate
Hexyl Acetate
Ethyl Hexanoate
Hexanol
Linalool
Geraniol
Phenylethyl alcohol
Citronellol
Hexyl cinnamal
Hexanal
Cis-3-Hexenol
Cis-3-Hexenyl acetate
Phenoxy acetic acid
Isobutyl acetate
Limonene
Citral
Phenylacetic acid
Decyl acetate
Naringin
Benzyl salicylate
Vetiverol
Santalol
Guaiacol
Trimethyl cyclohexene
Vanillin
Coumarin
Benzoin
Benzyl benzoate
Cinnamalde-hyde

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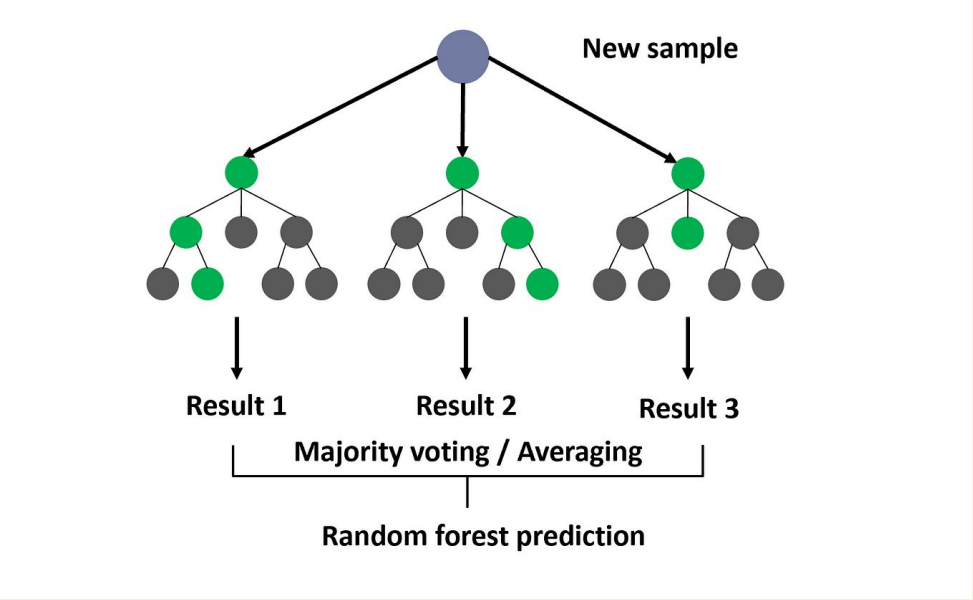
Random Forest



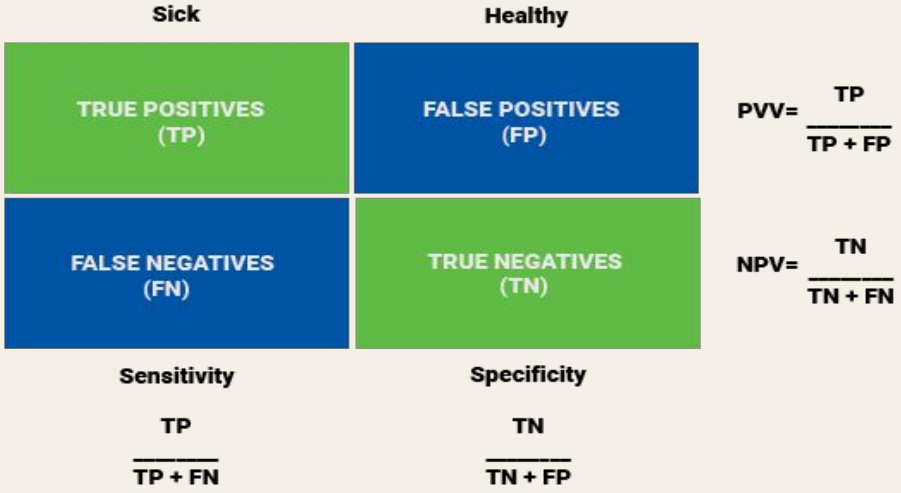

```
aroma_df[col].fillna(aroma_df[col].mean(), inplace=True)
              precision    recall  f1-score   support

      citrus       1.00      1.00      1.00        47
      floral       1.00      1.00      1.00        44
      fruity       1.00      1.00      1.00        45
       green       1.00      1.00      1.00        52
    oriental       1.00      1.00      1.00        36

    accuracy                           1.00       224
   macro avg       1.00      1.00      1.00       224
weighted avg       1.00      1.00      1.00       224

Cross-Validation Scores: [1. 1. 1. 1. 1.]
Mean Cross-Validation Score: 1.0
```

Future Direction



- Filtering OR from Cluster Heatmap
- More progress on ‘Random Forest’
- Measure Specificity / Sensitivity
- Color Aromatic Heatmap ligands based on their affinity
- involving multiple ligands or multiple receptors

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