

Pattern Analysis between OR and Six Categorized Aromatic Ligands

김명주 (**Bioinformatics**)

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



Visualization

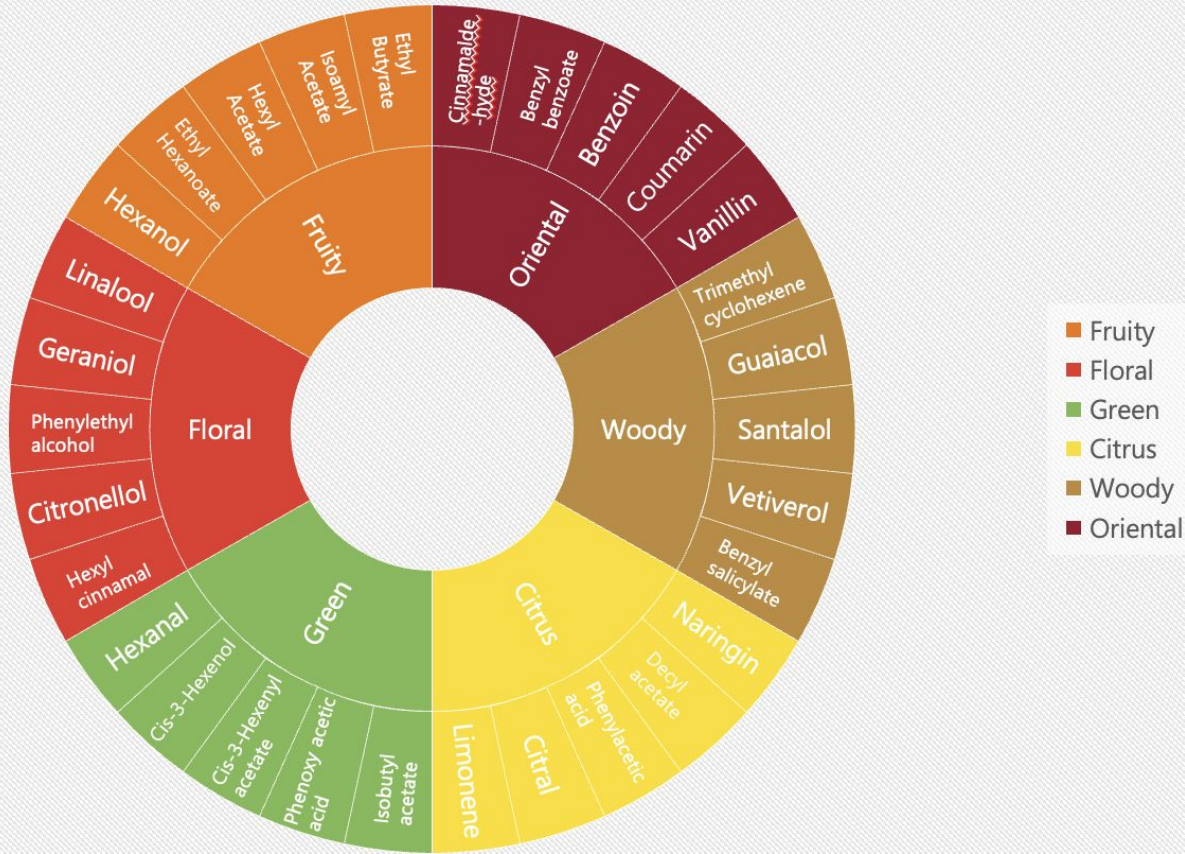
1. Citrus
 - a. largest affinity range between -4 and -10.
 - b. Similar trend ligand binding to ORs, beside Naringin
 - c. intuitively similar overall pattern with 'Green'
2. Floral
 - a. intuitively similar overall pattern with 'Fruity'
 - b. in terms of dendrogram of ligand, relates to 'Green'

3. Woody

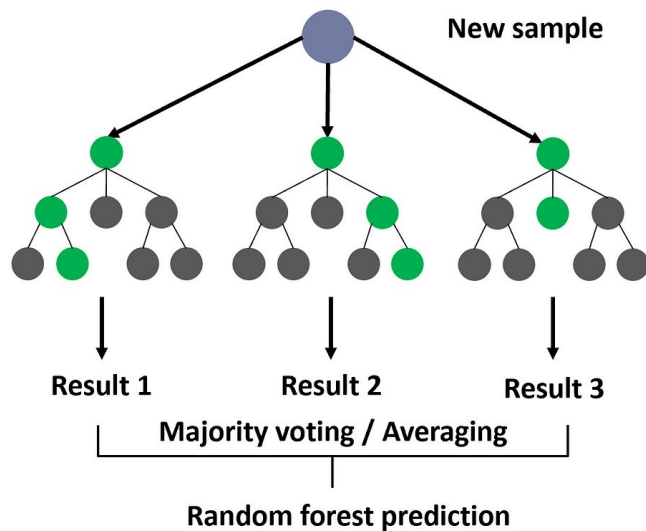
- a. intuitively mirrored overall pattern with 'Oriental'
- b. dendrogram reflects the relationship between 'Woody' and 'Oriental'

→ Overall reflects our Aromatic Wheel

Aromatic Wheel



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

