Gembloux Agro-Bio Tech
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Plant oxylipins: structure-function relationships

Arabidopsides

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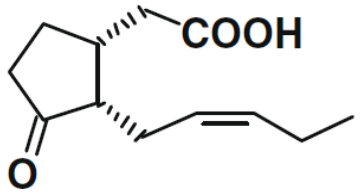
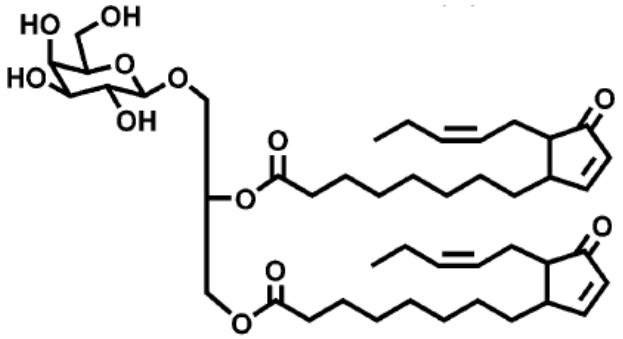
1. Context

- Plant oxylipins
  - Unsaturated fatty acids oxidation
  - Important roles
    - Biotic/abiotic stresses
  - Forms in plants
    - Free
    - Esterified
      - High diversity: galactolipids, phospholipids, …



Jasmonic acid



Arabidopside B

- Arabidopsides

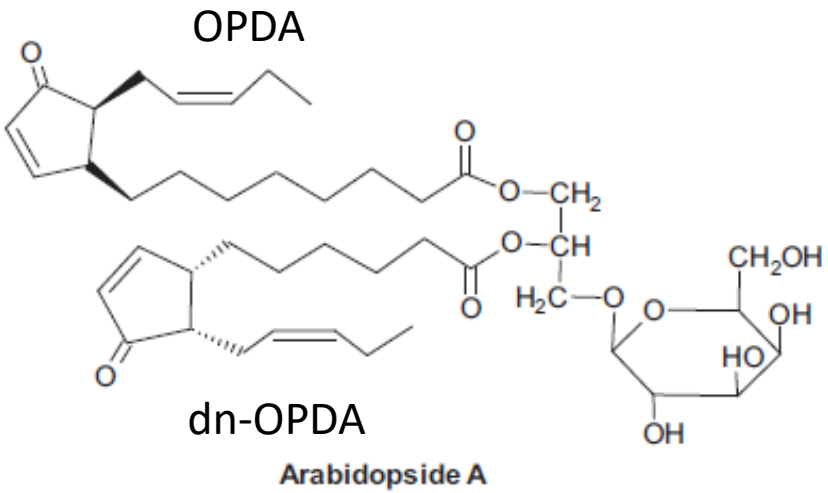
Stress

Wounding, cold, photoperiod, Bacteria pathogen

Arabidopsis thaliana L.

Arabidopsides production

- Same structure
- Found in few vegetal species



- Arabidopsides functions
  - Production following stress➔ plant defense mechanisms

Hypotheses

OPDA/ dn-OPDA supply

- Signaling pathway modulation
- For jasmonic acid production

Direct action on pathogens

- ↓ growth of *pseudomonas syringae (in-vitro)*

2. Project

- Goal: determination of arabidopsides involvement in plant defense mechanisms
  - Lipid molecules
    - Interact/found in plant membranes
  - Project
    - Purification of pure molecules
    - Study of molecules/membranes interaction *in-vitro* & *in-silico*

3. Results

1. Extraction of pure arabidopsides

$CHCl_3$:aceton (9:1)

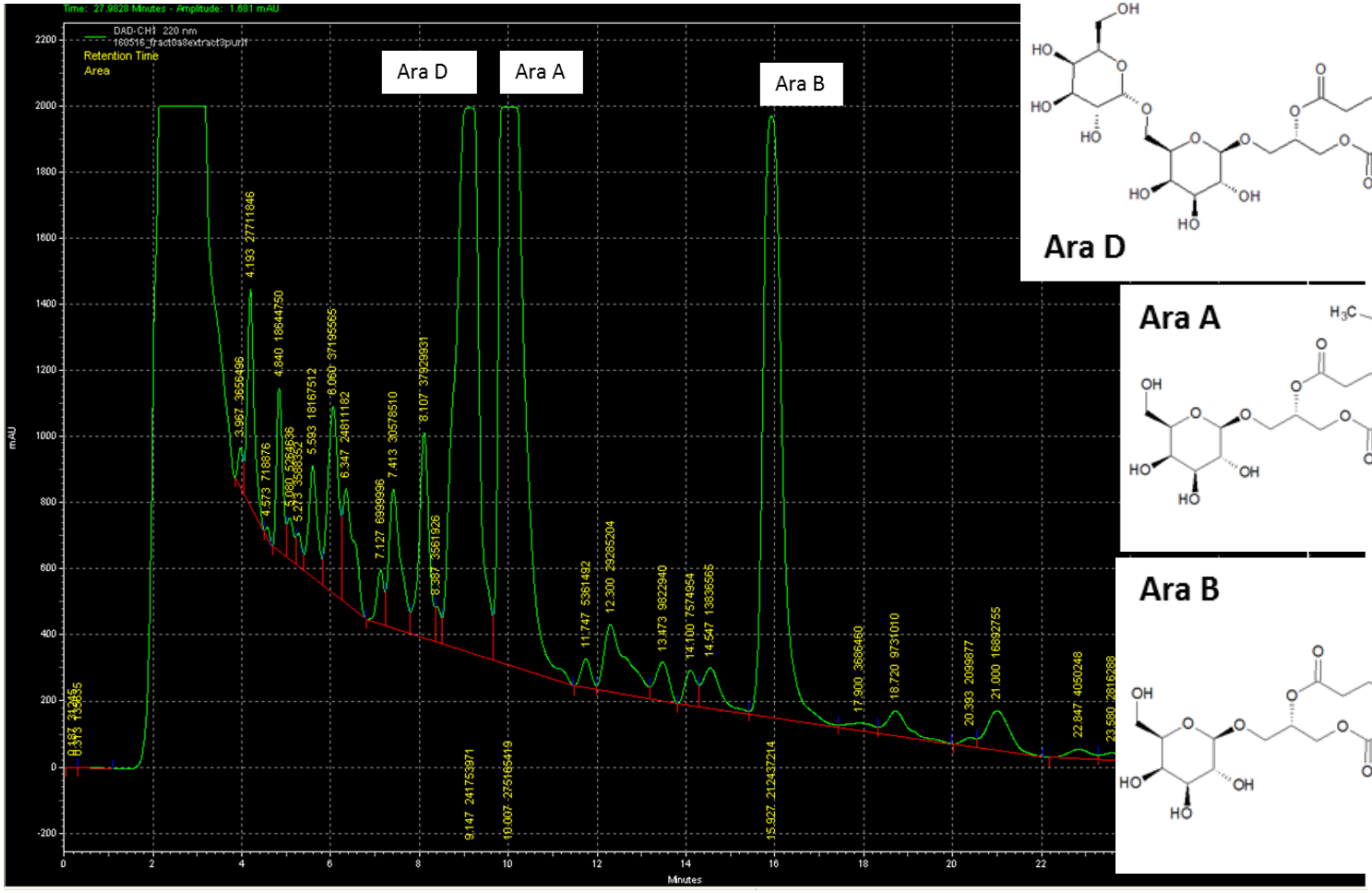
Aceto:methanol (9:1)

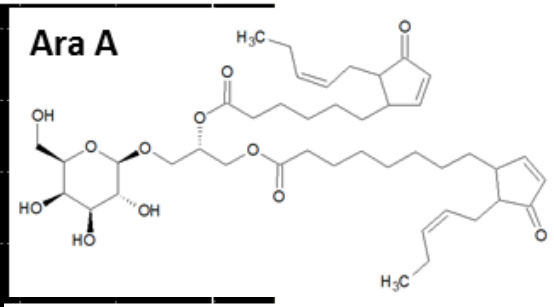
1. Apolar lipids
2. Glycolipids

Preparative HPLC Purification

- C18 column
- Acetonitril:water gradient
- UV detection

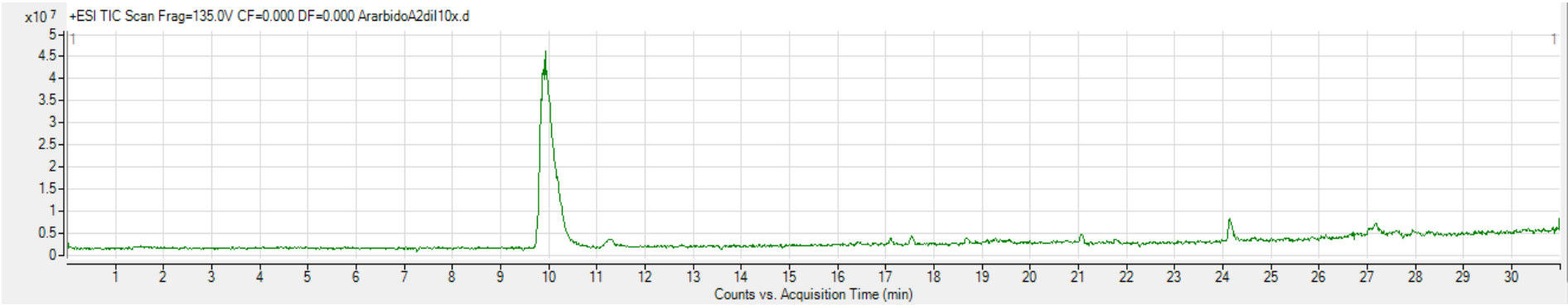
1. Extraction of pure arabidopsides

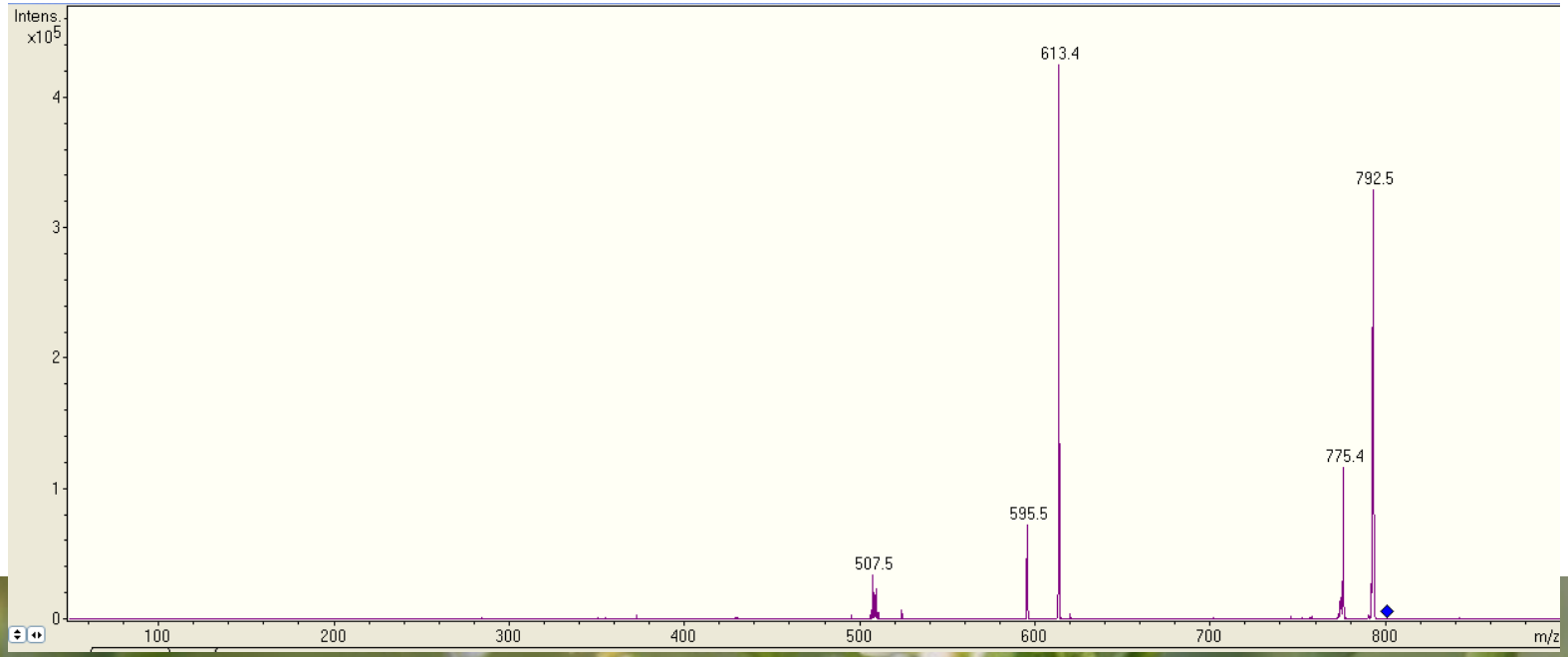




1. Extraction of pure arabidopsides

Arabidopside A





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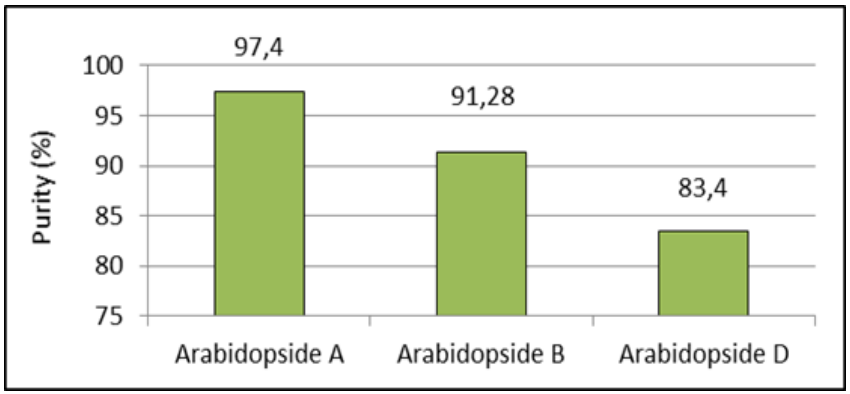
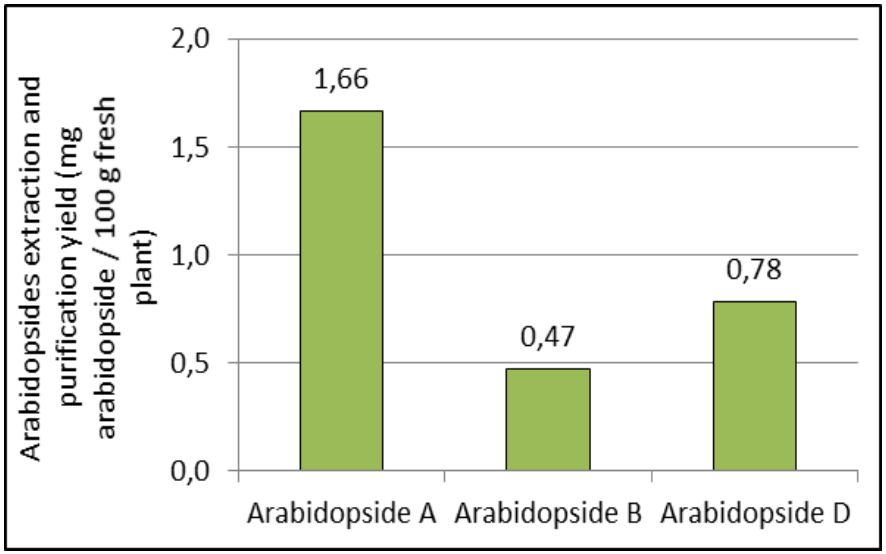
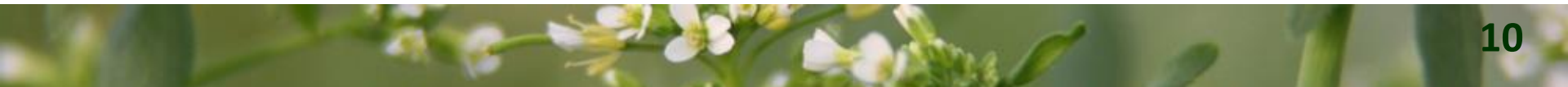




2. Arabidopsides *in-silic*o modelling

- Generation of **arabidopside A** 3D structures
  - 2 stereoisomers (R & S)

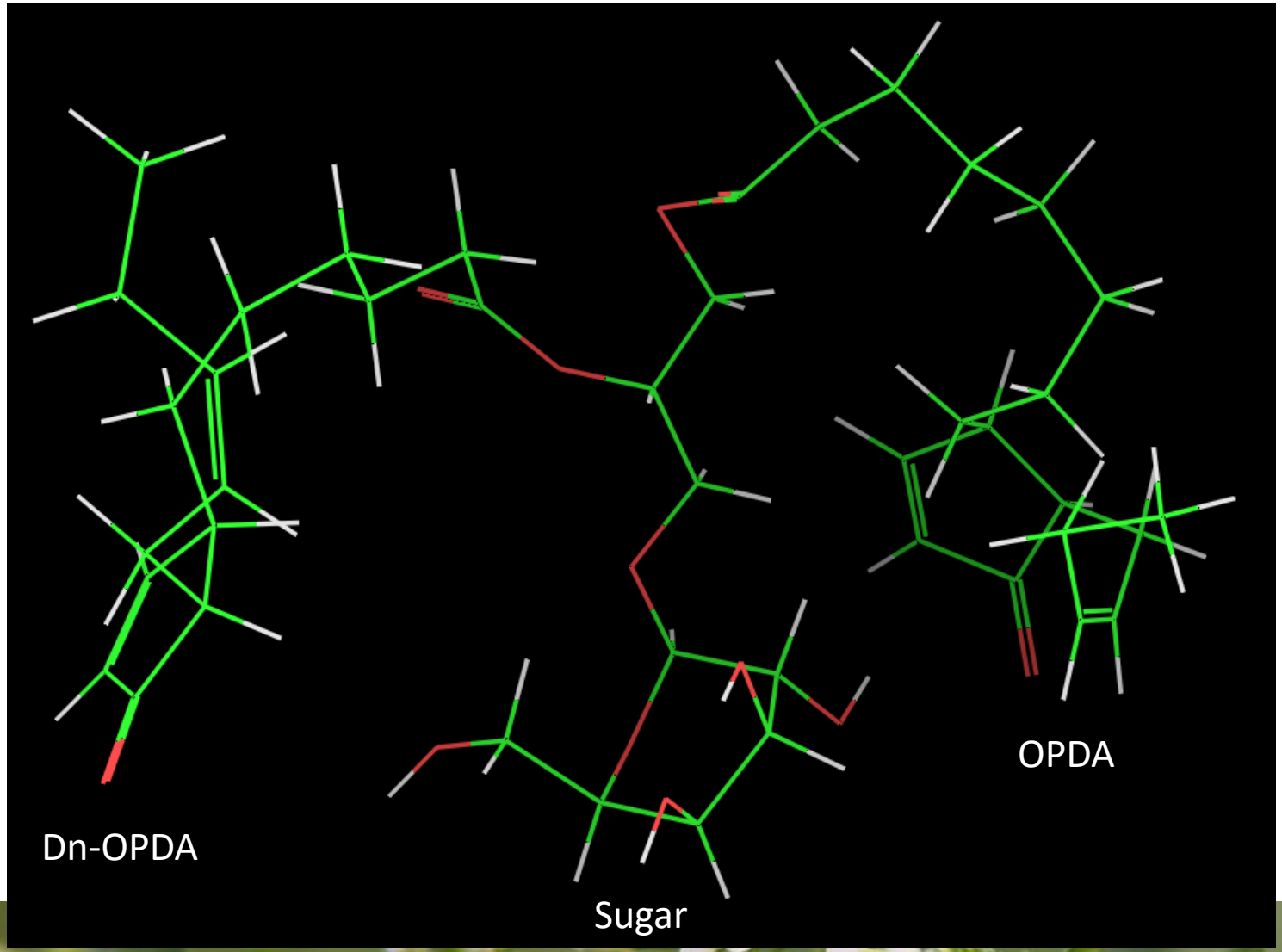


2. Arabidopsides *in-silico* modelling

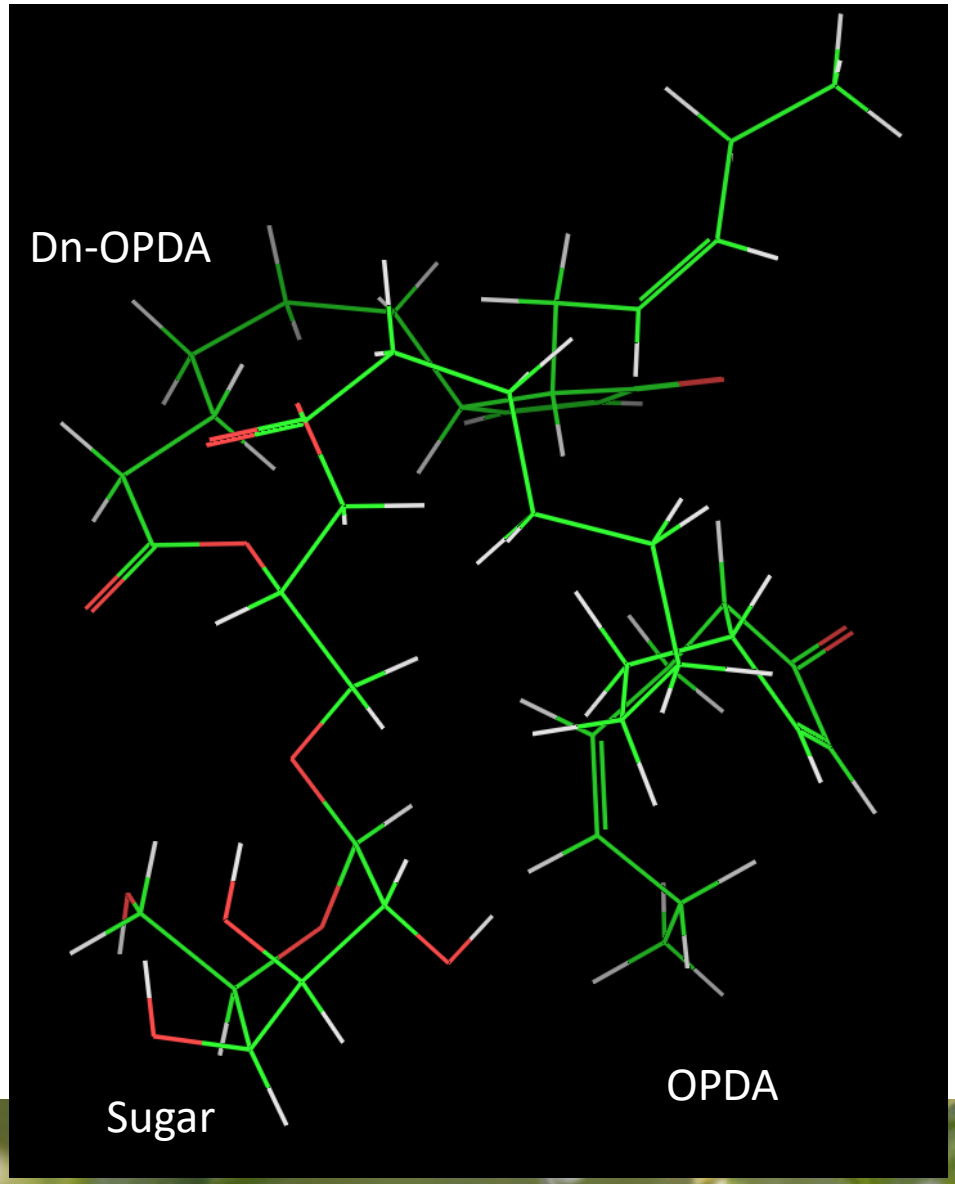
- Generation of **arabidopside A** 3D structures
- Structure Tree
  - Informatic tool
    - Structure optimization in force field
  - Generation of thousand structures based on molecules torsion axis
    - Lowest energy structure is selected for each stereoisomer

2. Arabidopsides *in-silico* modelling

R stereoisomer



2. Arabidopsides *in-silico* modelling

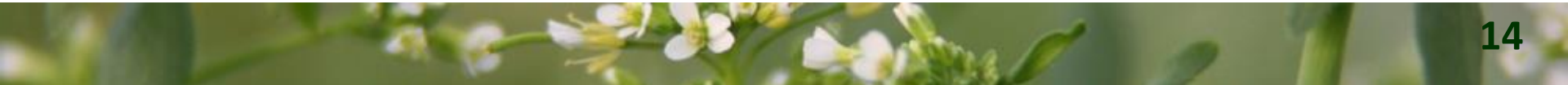


S stereoisomer

OPDA & dn-OPDA close

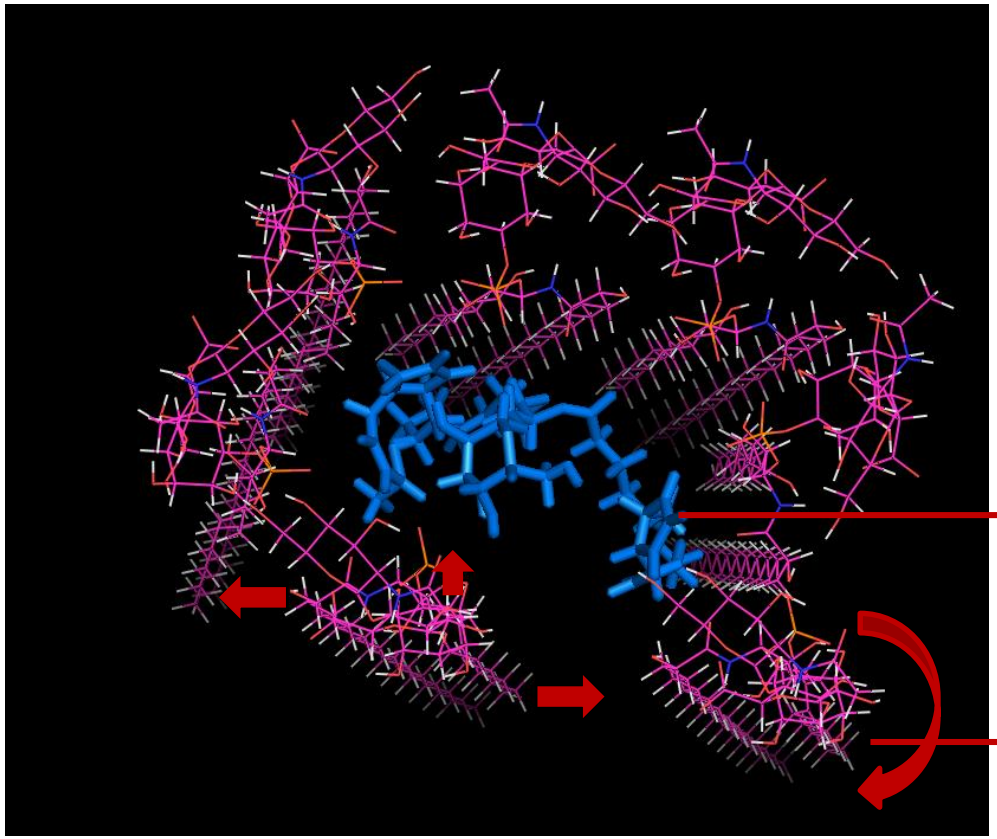
2. Arabidopsides *in-silico* modelling

- Generation of arabidopside A 3D structures
- Structure Tree
- Hypermatrix
  - Study interactions between
    - Interest molecules (structures generated before)
    - Plant membrane lipids (monolayer)



2. Arabidopsides *in-silico* modelling

- Hypermatrix



Fixed molecule

Lipids

- Rotation
- Favorable energy

Fixed molecule surrounded by lipids

Interaction energies calculated

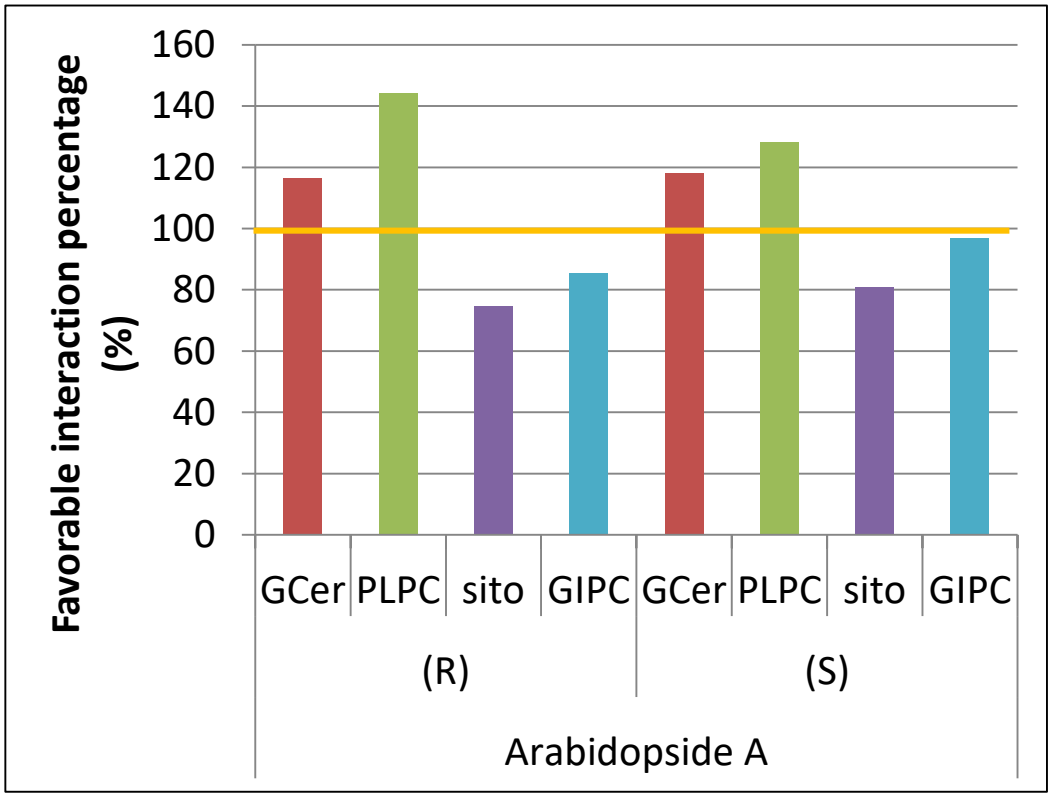
- Lipids /molecule/ lipids

Arabidopside A (R)

GIPC

2. Arabidopsides *in-silico* modelling

- Hypermatrix: interaction energies
  - Surrounding arabidopsides lipids energies compared to monomolecular lipids energies



GCer and PLPC: Favorable

Sito and GIPC: No favorable

PLPC: (R) more favorable than (S)

4. Conclusion

- Arabidopsides can be extracted and purified from stressed plants
- *In-silico* simulations
  - Arabidopsides can positively interact with plant plasma membrane lipids
- Perspectives
  - *In-vitro* analysis
    - E.g: are arabidopsides able to permeabilize plant membranes?

Thank you for your attention