



HAL
open science

Modulation of Spirulina extraction using Natural Deep Eutectic Solvents with respect to predicted thermodynamic properties

Mervé Yagmur, Alia Chevalley, Bénédicte Montigny, Johan Jacquemin, Leslie Boudesocque-Delaye

► To cite this version:

Mervé Yagmur, Alia Chevalley, Bénédicte Montigny, Johan Jacquemin, Leslie Boudesocque-Delaye. Modulation of Spirulina extraction using Natural Deep Eutectic Solvents with respect to predicted thermodynamic properties. Cosm'Innov International Congress, May 2023, Orléans, France. <hal-04951827>

HAL Id: hal-04951827

<https://hal.science/hal-04951827v1>

Submitted on 17 Feb 2025

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

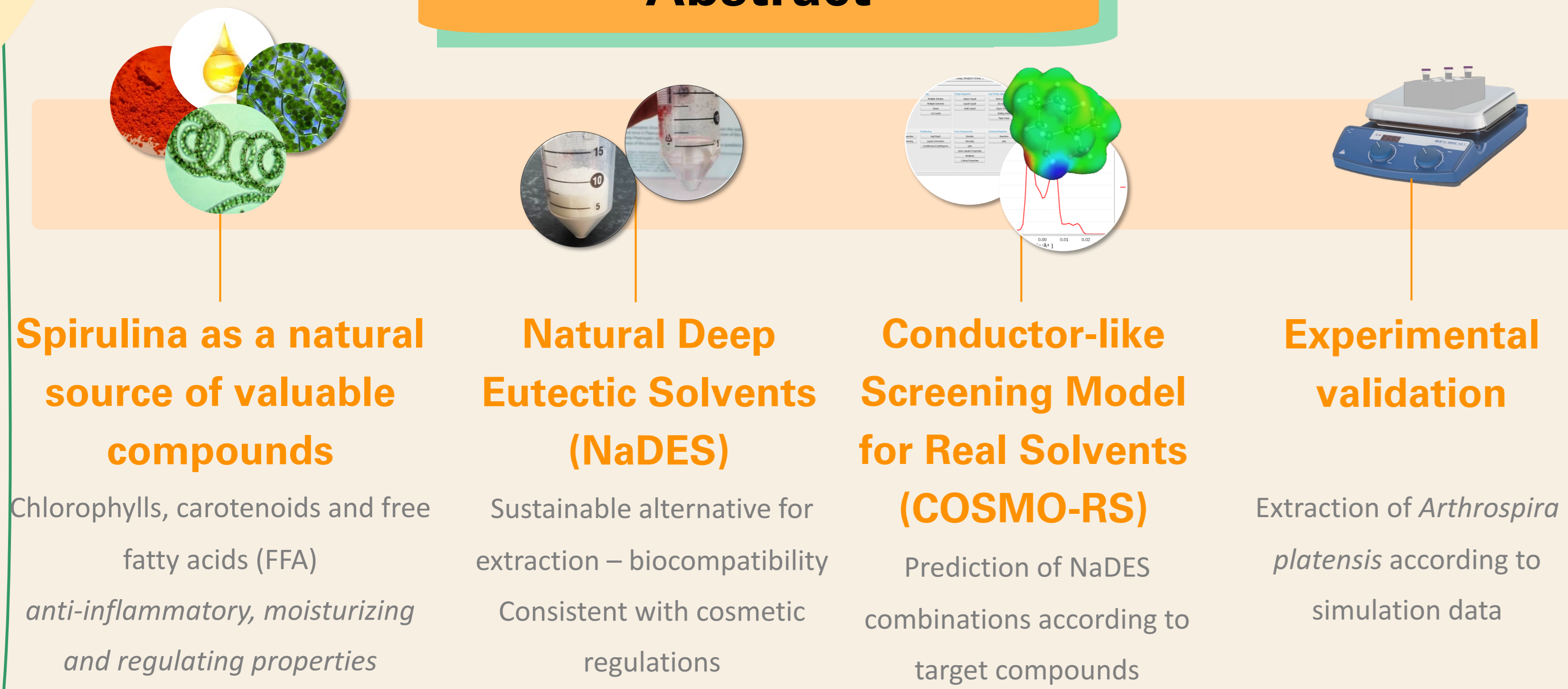
L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



HAL Authorization

Modulation of Spirulina extraction using Natural Deep Eutectic Solvents with respect to predicted thermodynamic properties

Abstract



Objectives

- Prediction of:**
- The best NaDES combination for selective extraction
 - The most effective molar ratio

Simulation tools

Experimental

- Confirm theory with practice
- Comparison of different ratios

- Development of a new routine methodology for the laboratory

Methodology

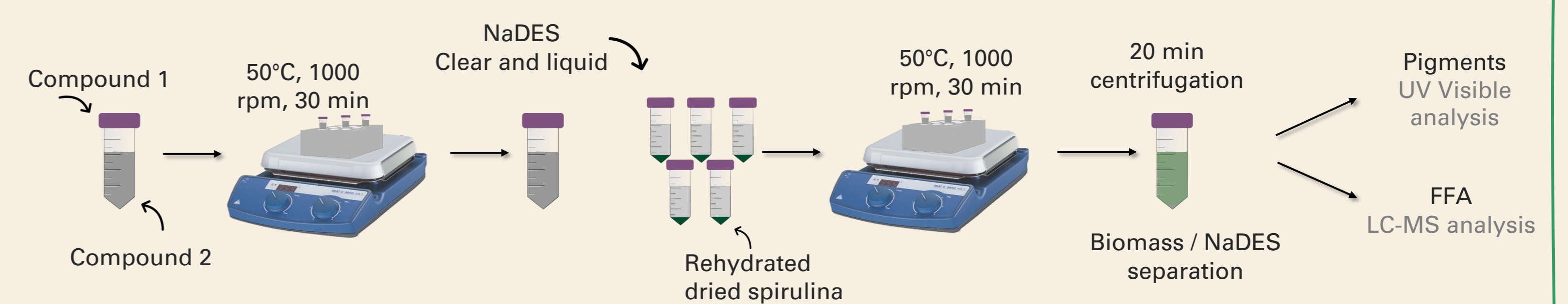
Methods

COSMO-RS

The screening for different NaDES combination according to target compounds structures was performed using COSMOthermX (2021) software.

The sigma profiles and potentials, as well as the solid-liquid equilibrium (SLE) to determine the eutectic point of each NaDES, were described through the same software.

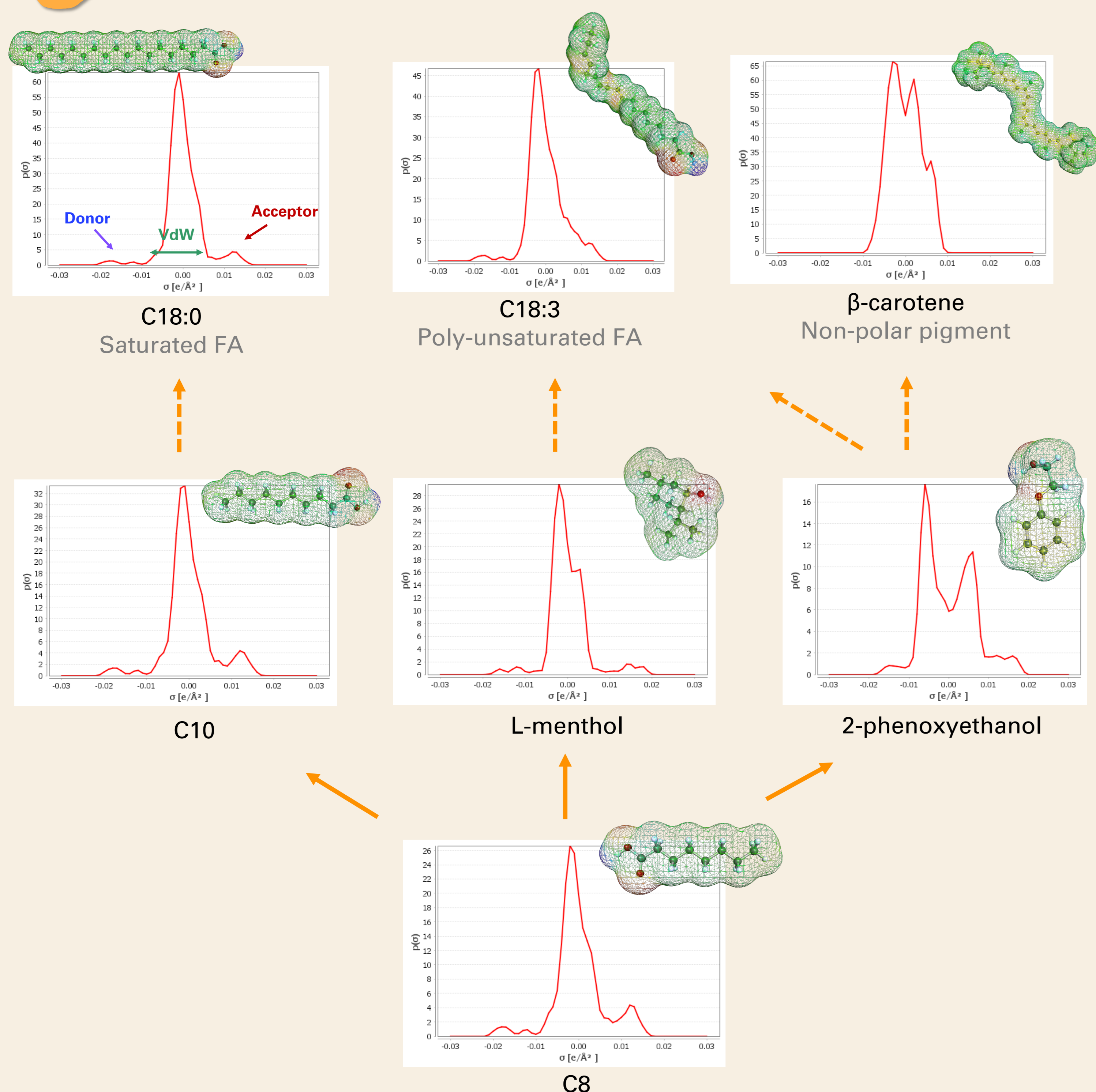
EXPERIMENTAL



The dry biomass was rehydrated prior to the extraction process for reproducibility

Results

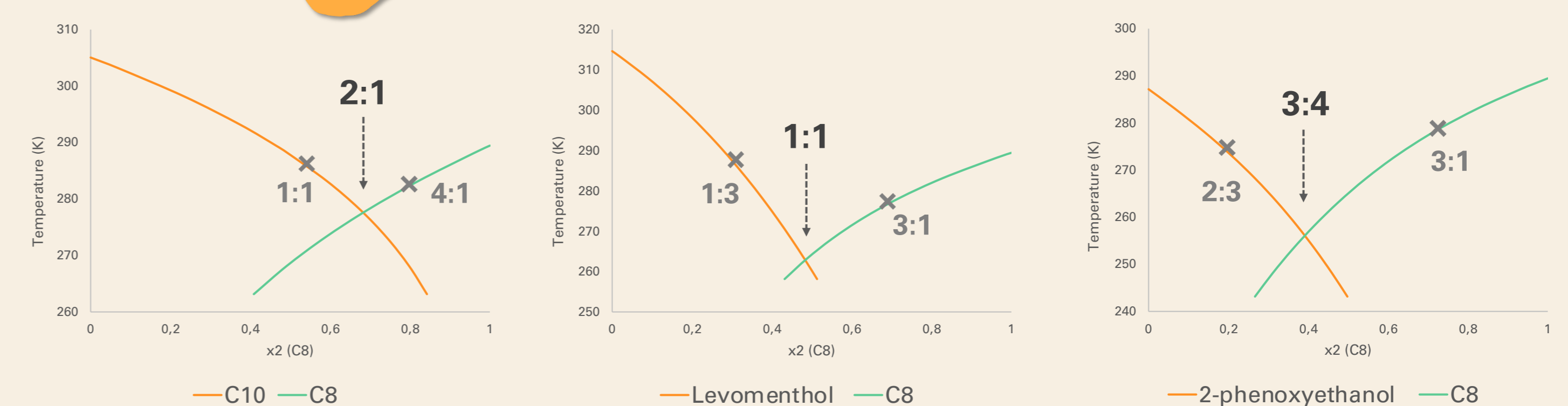
1 3 CATEGORIES OF TARGET COMPOUNDS



2 NaDES COMBINATIONS

Octaoc acid (C8) was selected as a common structure for each NaDES combination for its high FFA extraction capacity [1].

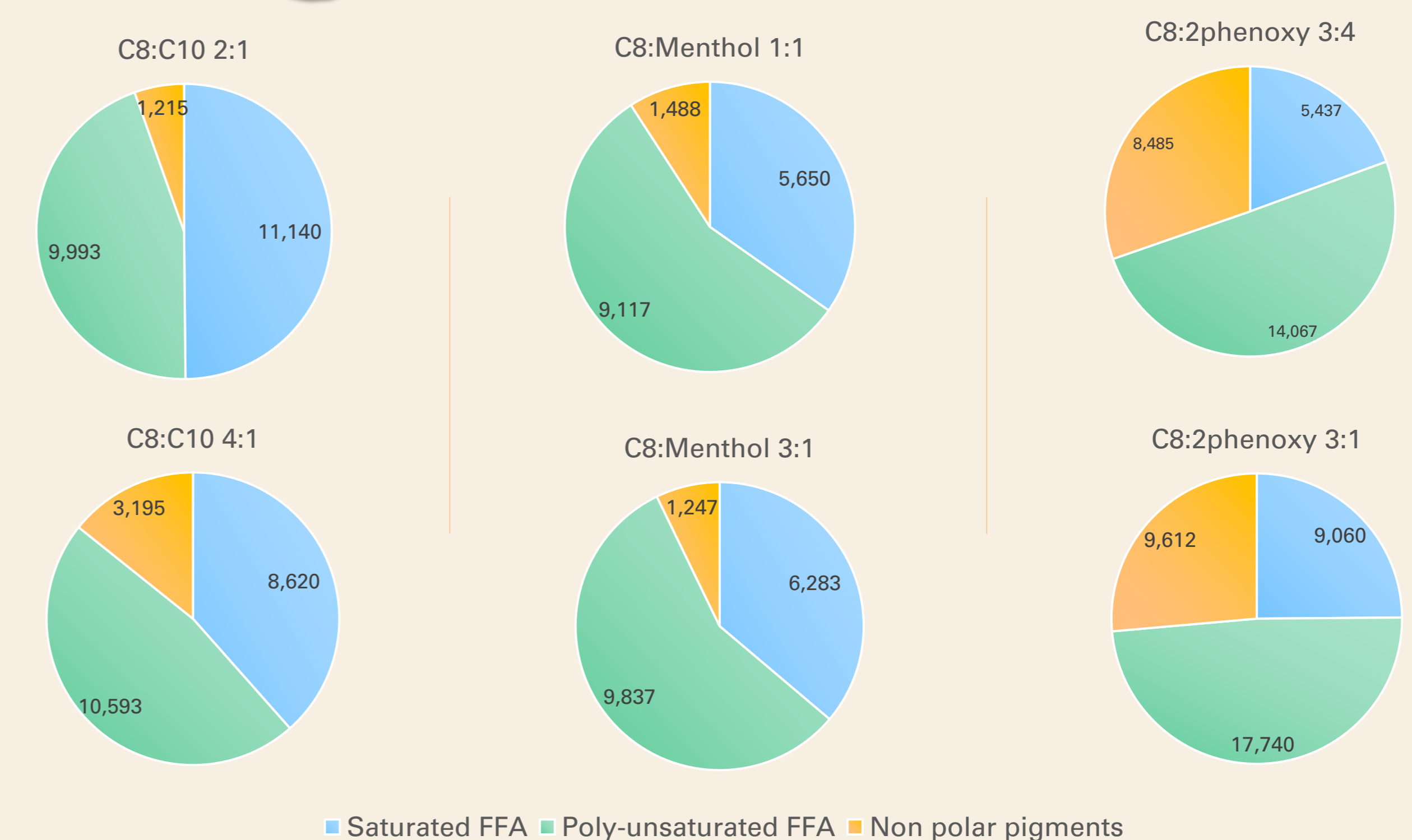
3 EUTECTIC POINT DETERMINATION



The SLE determination for each combination allowed estimation of the eutectic ratio (dark grey).

For each NaDES, two other molar ratios were selected to experimentally evaluate the effect of C8 amount in each mixtures (light grey).

4 EXPERIMENTAL DATA



These diagrams represent the 3 groups of target compounds for the different mixtures. The results are presented only for the eutectic ratios and C8 rich ratios.

The values in each section corresponds to the amount of mg of targeted compounds per g of dry matter.

Conclusions

According to the **screening on COSMO-RS**, the use of some mixtures seems preferable to target the different compounds one can find in Spirulina:

- C8 associated with C10 is most likely preferable for saturated FFA extraction
- C8:2-phenoxyethanol would be more suitable for unsaturated FFA or pigments extraction due to charge delocalization
- C8:Menthol seems preferable for both type of FFA extraction

- C8:2-phenoxyethanol helps increasing the amount of non-polar pigments and poly-unsaturated FFA
- C8:Menthol extracts are in an intermediate state
- The amount of C8 have a variable effect on target compounds extraction depending on the second compound of the mixture

➔ This work will help us to go further in **selective extraction** of some compound to minimize the amount of the non-targeted compound categories.

Experimentally, as we expected:

- C8:C10 has a higher amount of saturated FFA