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## **COSMO-RS as a cutting-edge technology for designing and pre-screening of Natural Deep Eutectic Solvents for selective extraction: Spirulina as a case study**

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# COSMO-RS as a cutting-edge technology for designing and pre-screening of Natural Deep Eutectic Solvents for selective extraction: Spirulina as a case study

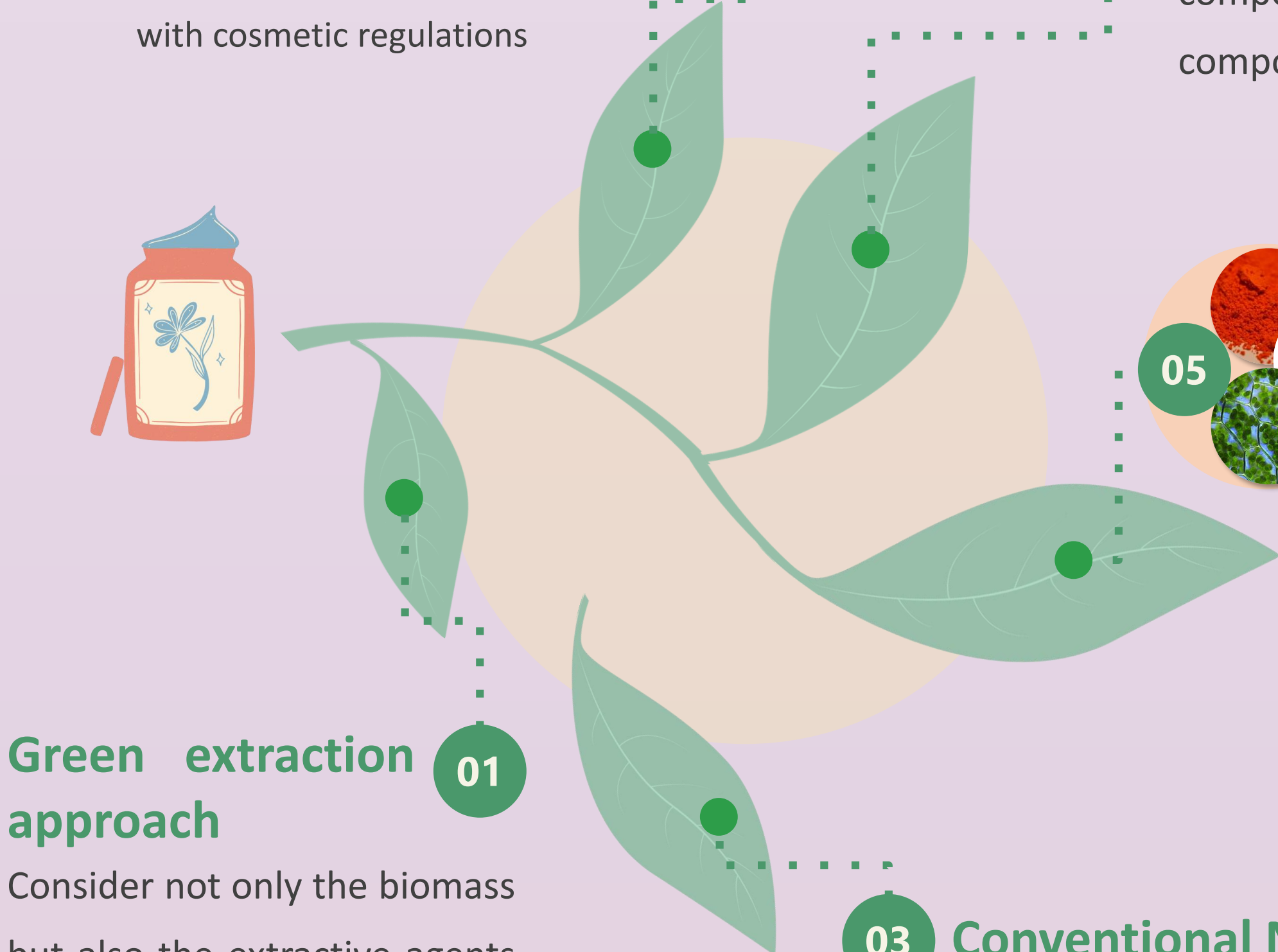
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## Introduction

### NaDES as designer solvents

**Natural Deep Eutectic Solvents** – Sustainable alternative for targeted extraction process and compatible with cosmetic regulations



### Green extraction approach

Consider not only the biomass but also the extractive agents used at each step of the overall process

### Conventional NaDES conception

Experimental screening of different ratios: a time- and solvent-consuming process

### COSMO-RS as a screening tool

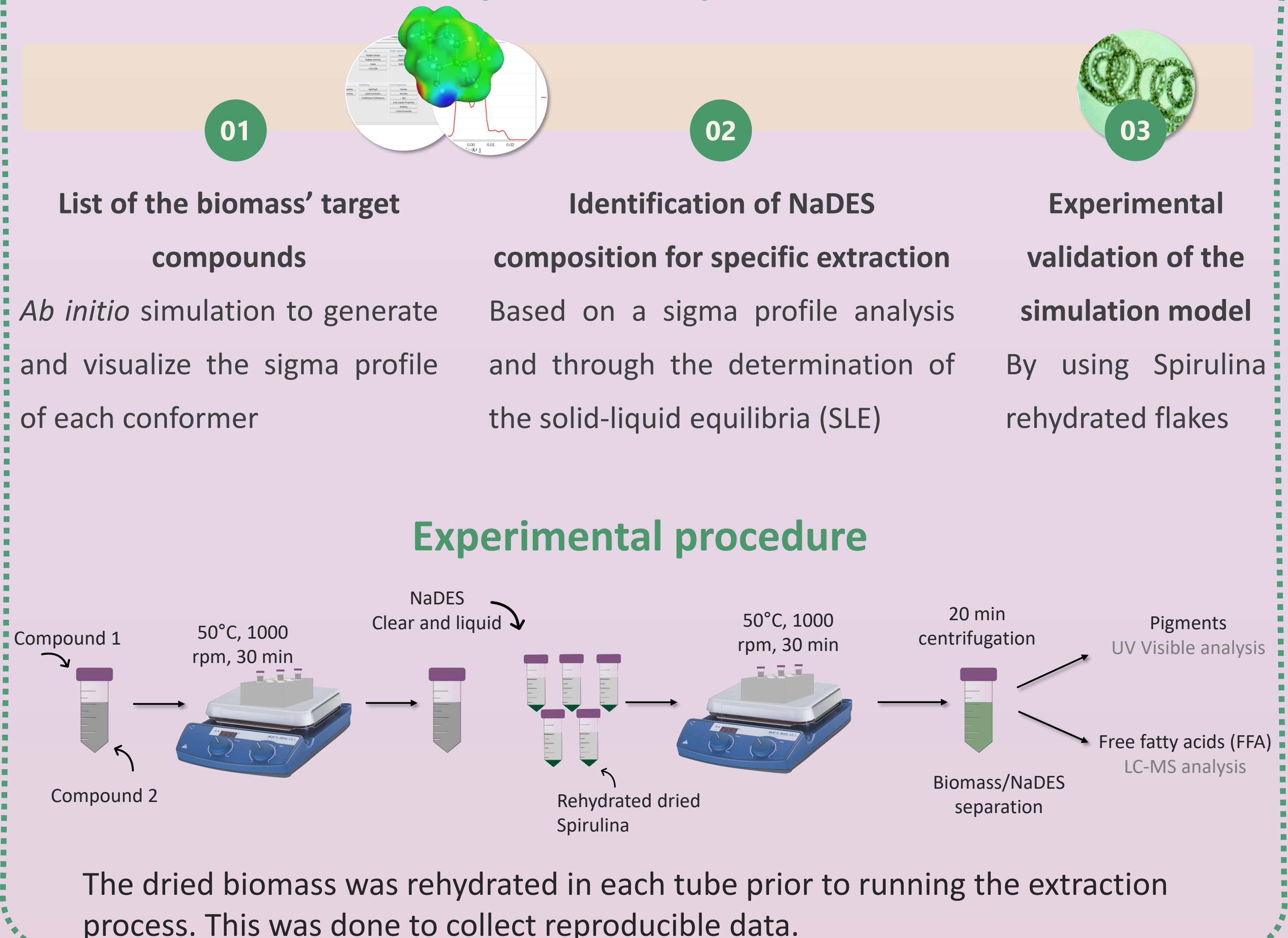
**COnductor like Screening MOdel for Real Solvents** – Identification of NaDES composition according to targeted compounds

### Arthrospira platensis used as a probe

- *In silico* screening of potential NaDES for selectively extracting targeted high-value compounds  
- Experimental validation  
- Eutectic window

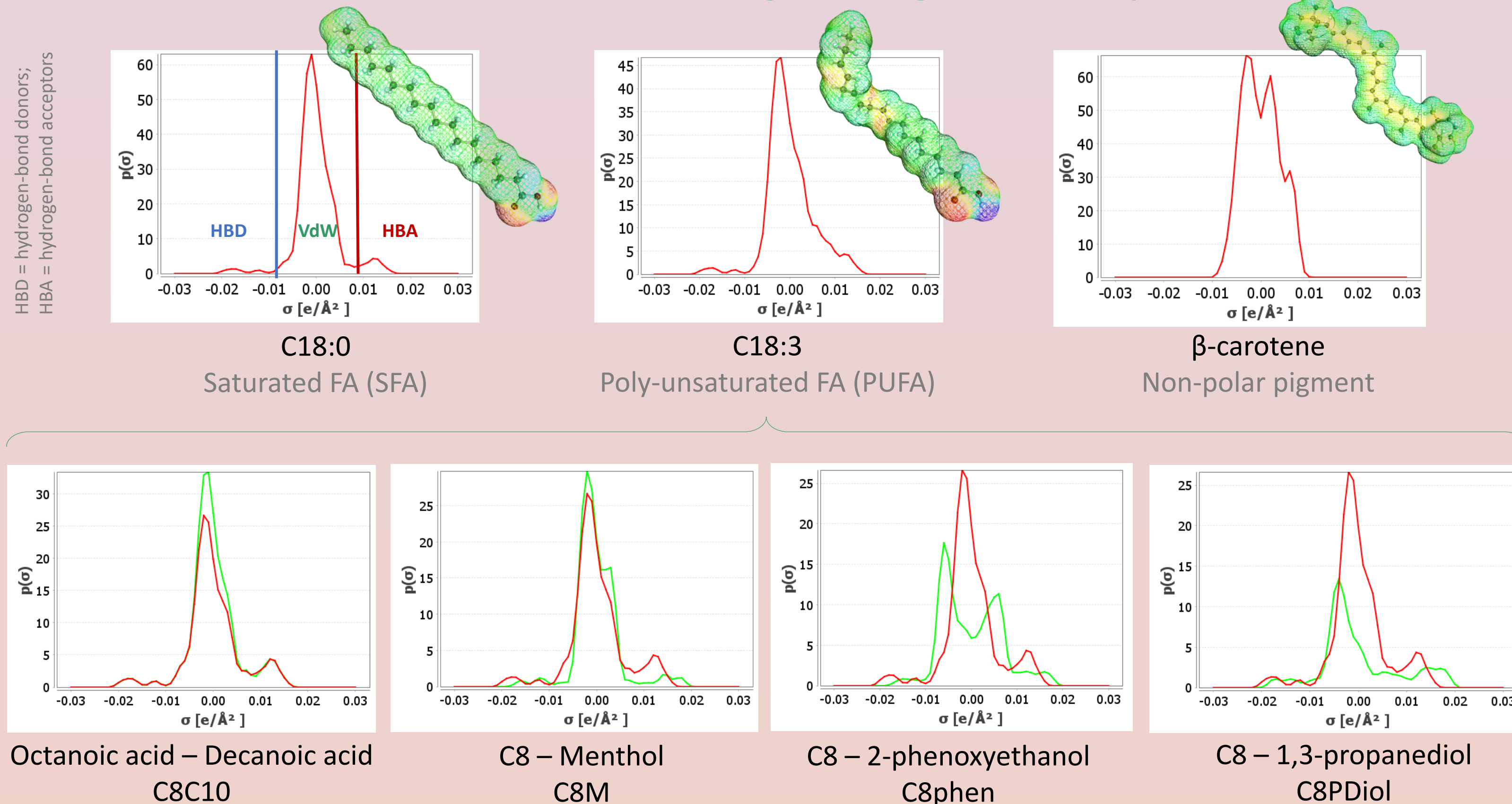
## Applied methodology

### Comprehensive procedure



## Simulation for extractive solvent selection

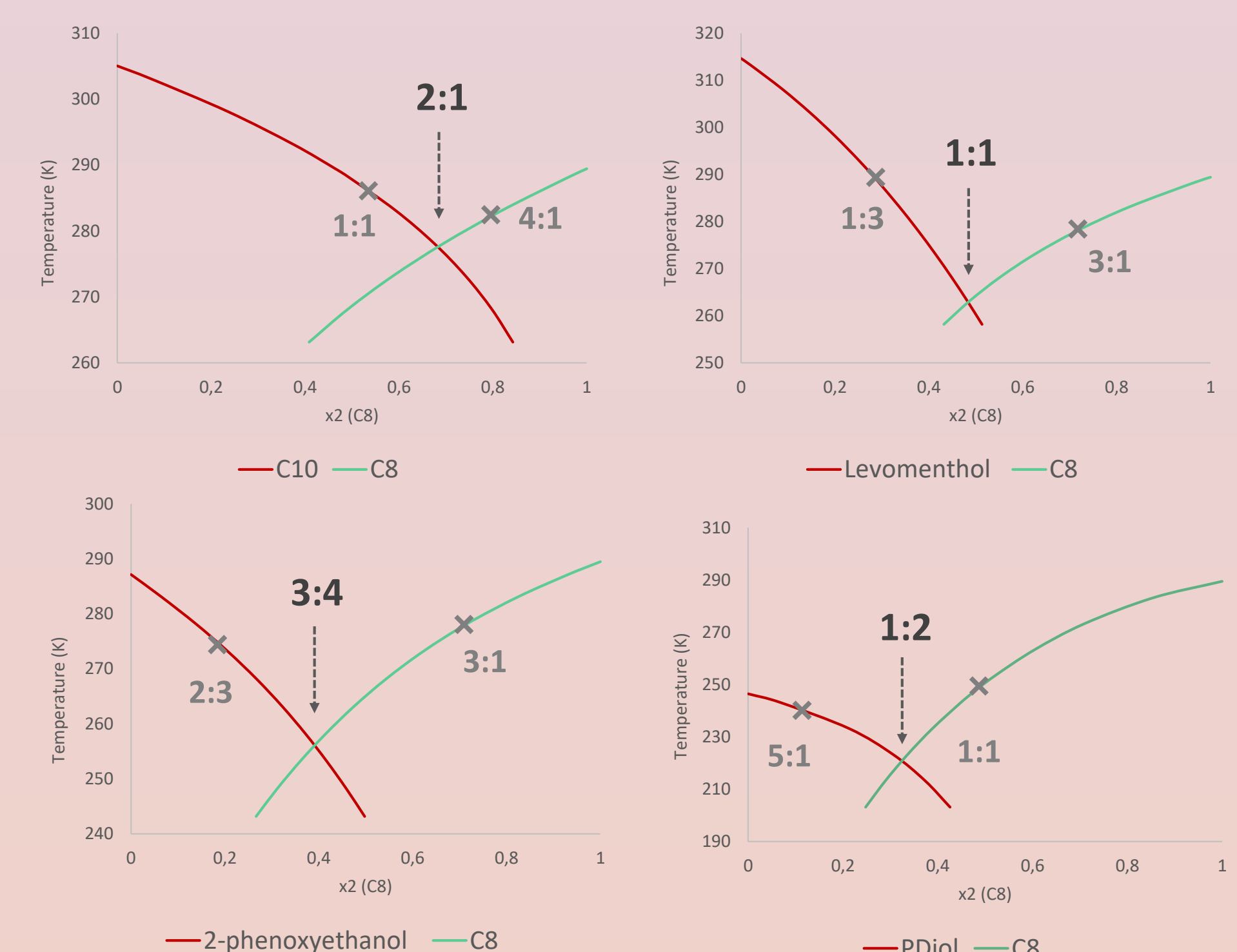
### Selected NaDES according to targeted compounds



C8 was selected for each NaDES combination based on its high FFA extraction capacity.<sup>1</sup> Co-solvents were chosen based on the complementarity of their sigma profiles with C8. This strategy was also used during the *in silico* screening of NaDES formulation to efficiently extract target compounds.

### Eutectic point determination

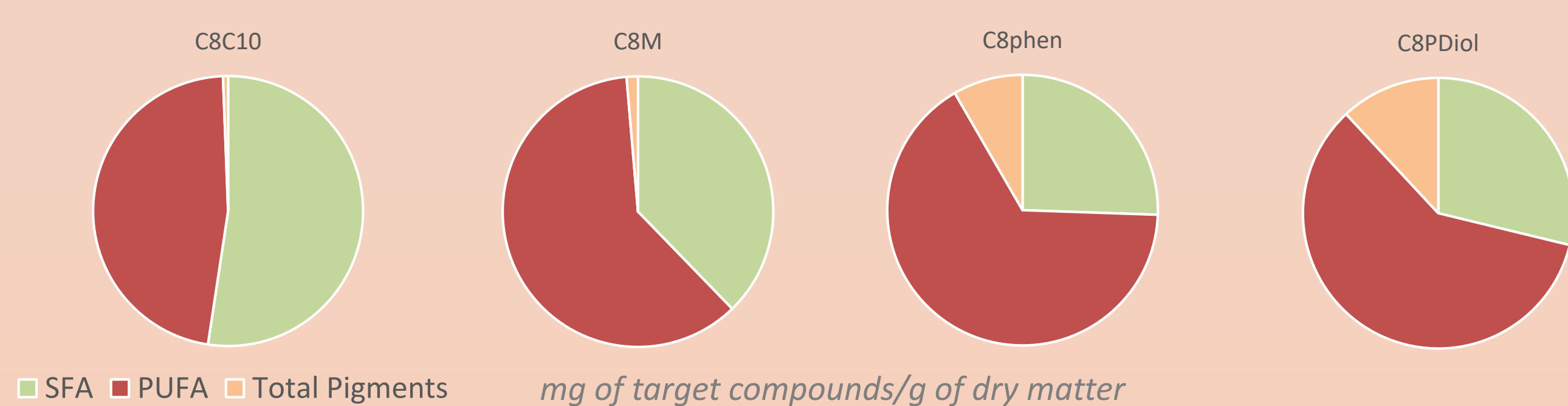
The SLE determination allowed estimation of each eutectic ratios (dark grey).



For each NaDES, two additional molar ratios were also investigated to experimentally evaluate the effect of the extractant formulation on the process selectivity toward targeted compounds (light grey).

## Experimental results

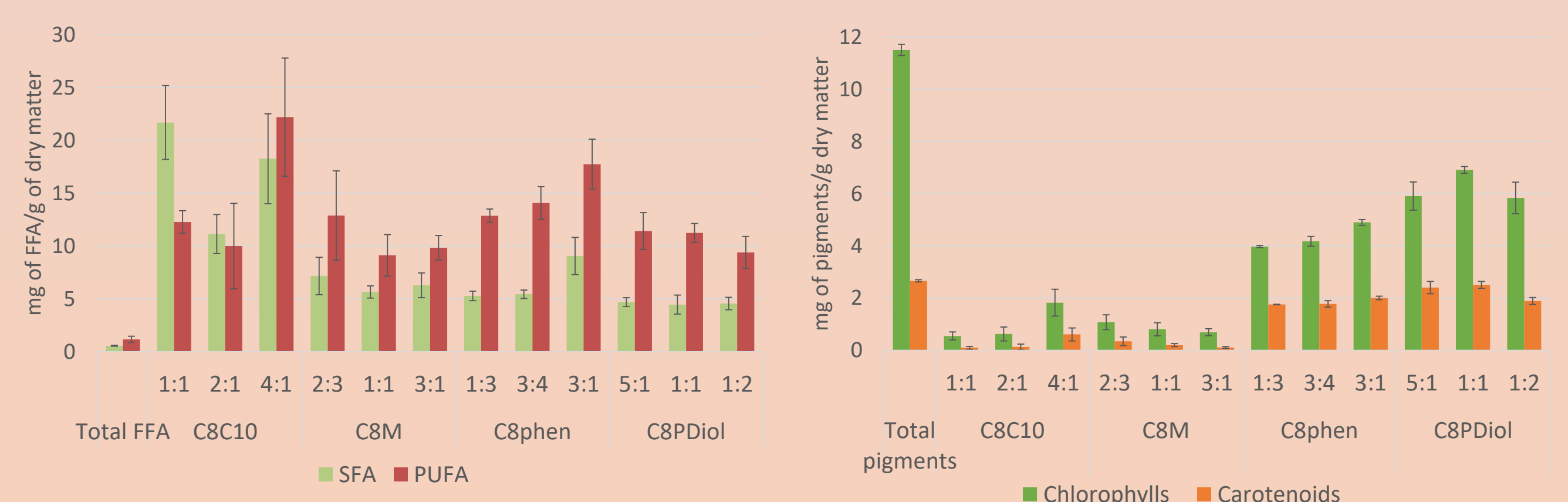
### Evaluation of the *in silico* NaDES selection



These diagrams represent the 3 groups of target compounds for the different mixtures at the eutectic ratios.

✓ The experimental results are consistent with the simulation hypothesis.

### Effect of the extractant formulation



The extractant formulation must be fine-tuned to reach a selective extraction of a specific compound. Eutectic compositions are often less effective due to strong interactions between the solvent molecules.

## Conclusions and perspectives

### A driver to extract nonpolar compounds from Spirulina:

#### Screening done according to COSMO-RS to reach high selectivity

- **SFA:** C8C10 most likely preferable
- **PUFA:** C8M; C8phen & C8PDiol
- **Pigments:** C8phen & C8PDiol due to charge delocalization

#### Experimentally:

- C8C10 has a higher extraction potential for SFA
- Both C8phen and C8PDiol could be used to extract nonpolar pigments and PUFA
- C8M is interesting for extracting PUFA with a low pigments content

### Eutectic effect

- Each eutectic point was determined by computing the SLE using COSMO-RS
- Eutectic composition is not always the best to be used when formulating a NaDES
- The extraction capability and selectivity can be optimized by using the sigma profiles of solvents along with their ratios to be used as extractant based on calculated SLE

### Perspectives

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

