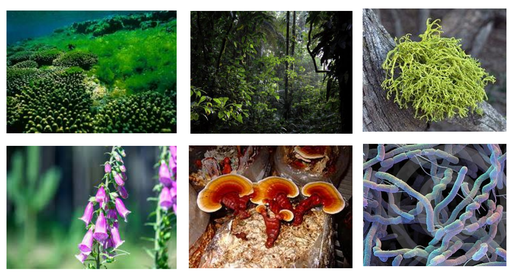
CARAMEL – A robust analytical strategy to support R&D in the cosmetic industry for the chemical profiling of natural ingredients

Alexis Kotland, Joseph Thiery, Pierre Darme, Jane Hubert
NatExplore SAS, Reims, France

The cosmetic sector is continuously evolving towards a much wider use of natural ingredients. There are today so many possibilities ! Not only in terms of resources, from terrestrial plants to marine species, fungi, bacteria, or other microorganisms, but also in terms of green solvent opportunities and extraction processes. The resulting ingredients exhibit sometimes extraordinary chemical profiles, often highly complex. Such profiles must be carefully assessed with an overall and deep approach.

The CARAMEL strategy relies on a unique analytical workflow, which combines different technologies providing each key advantages to determine the chemical composition of natural extracts:



NATURAL EXTRACT

Terrestrial, marine, microbial origin…

All types of extracts: Dry powder; Evaporable liquid extract (H_2O, EtOH…); "Heavy" solvents (glycerol, propanediol, butanediol…); NADES extracts

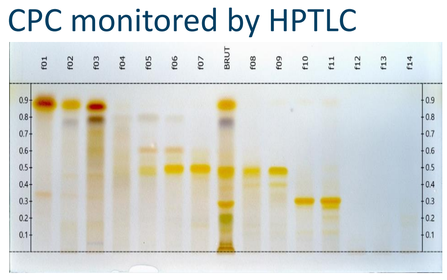
Liquid-liquid fractionation (Optional) to remove support/solvent or to separate abundant primary metabolites (fatty acids, simple sugars, salts) from more specialized metabolites

GILSON

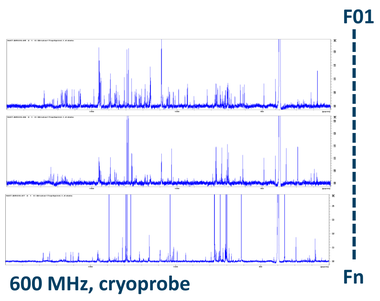
CENTRIFUGAL PARTITION CHROMATOGRAPHY

No loss of biomass
➔ Full extract recovery

CPC monitored by HPTLC



SPECTRAL ANALYSES

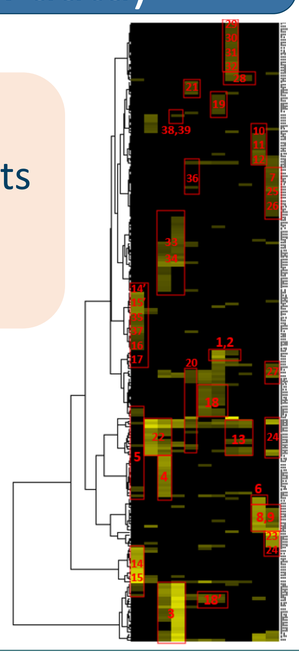


BRUKER

NMR (on all CPC fractions) + LC/MS (on the crude extract)

- **NMR**: Detection of organic molecules; No discrimination between chemical classes; Peak intensity proportional to metabolite concentration
- Metabolite annotation by **LC/HRMS:** Complementary to the NMR identification process

HIERARCHICAL CLUSTERING (on ^{13}C NMR data)



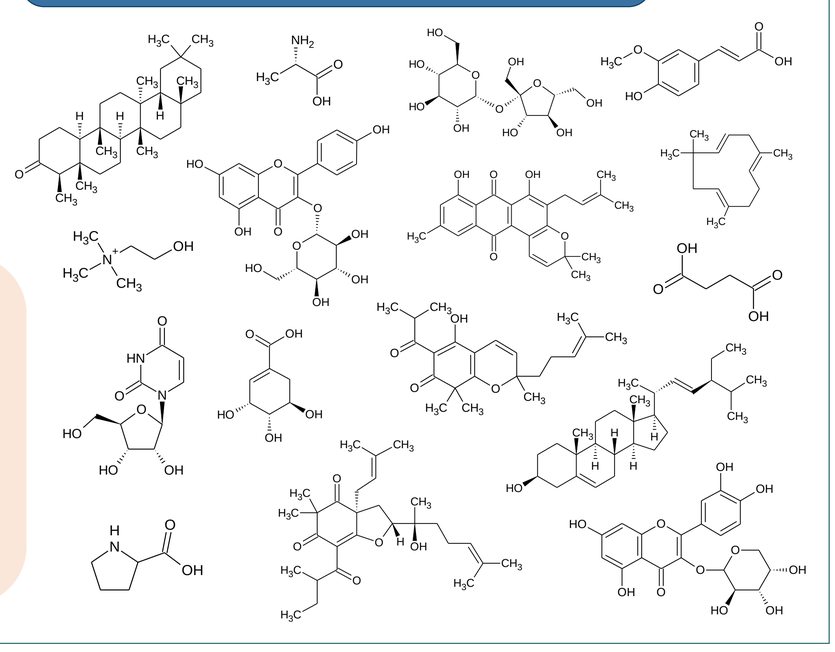
DATABASE

ACD/Labs

C+H

NMR database (predicted δ ppm)
- From ^{13}C clusters to chemical structures
- All atoms and correlations validated by rigorous interpretation of 2D NMR data
- Further elucidation of unknown compounds

METABOLITE IDENTIFICATION



- **Extract mapping**
- Similarity measurements
- **Carbon fingerprints of extract constituents**

⇒ **Time, solvents, and cost saving for the chemical profiling of natural ingredients;**
⇒ **Assistance in the determination of which compounds are involved in a biological activity;**
⇒ **CARAMEL is not destructive: at the end of the identification process, all fractions are dried and returned to our partners for biological / toxicological evaluation or complementary analyses.**

NATEXPLORE SAS (+33) 06 19 02 75 06 / contact@nat-explore.com / www.nat-explore.com