

Amélioration de la calibration d'un spectromètre visible grâce à la simulation optique

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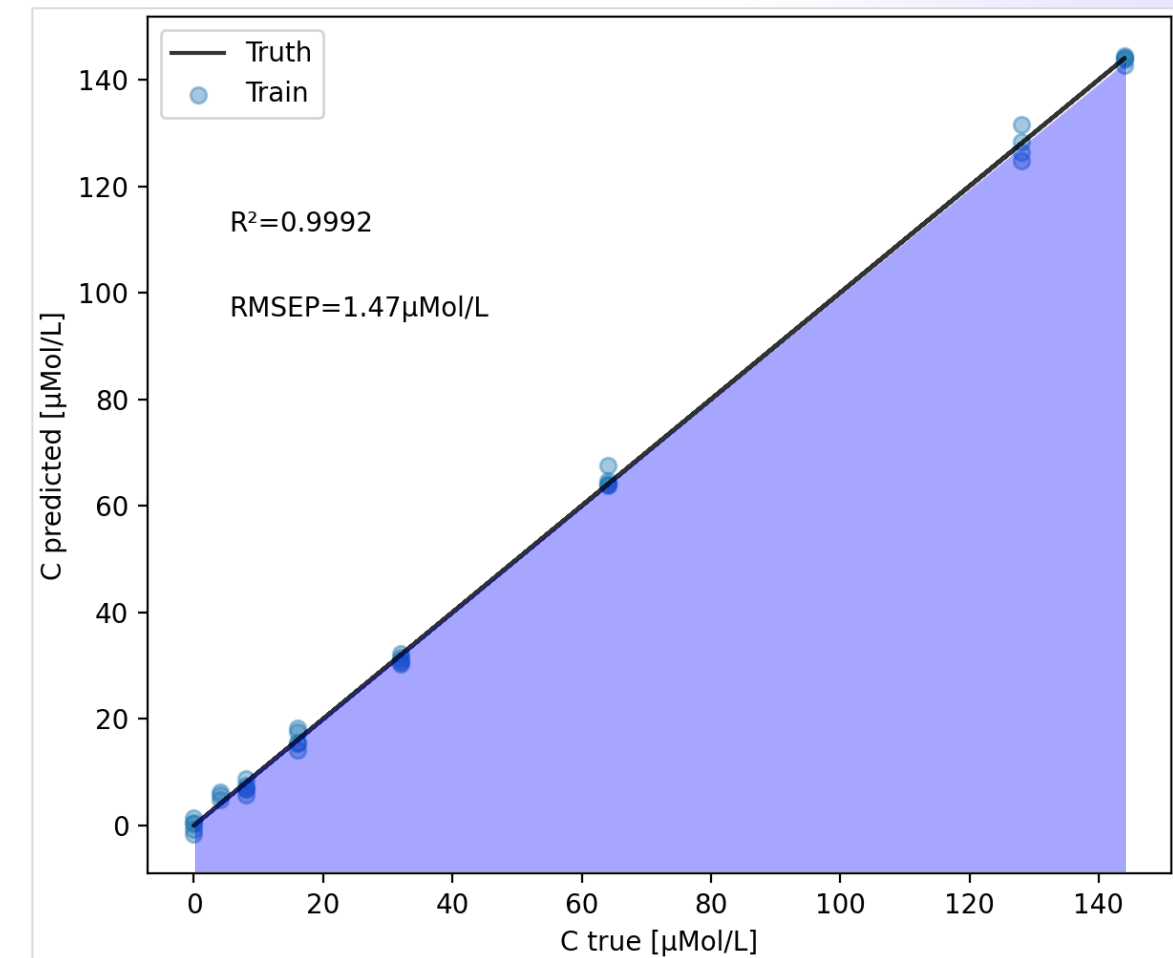
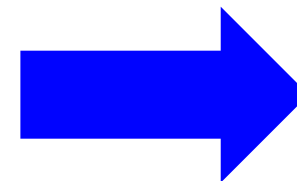
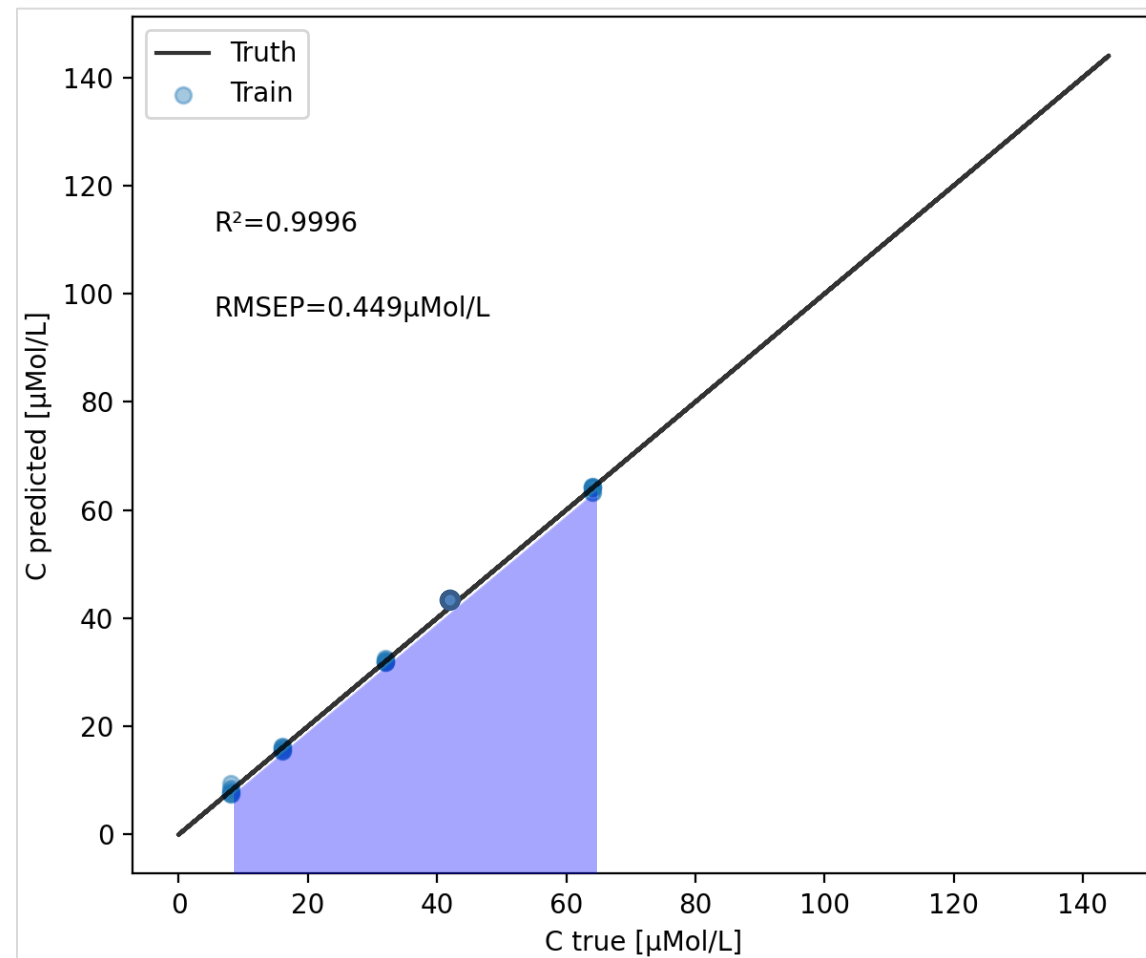
¹INRAE Montpellier, ITAP

²Indatech, Chauvin-Arnoux Group

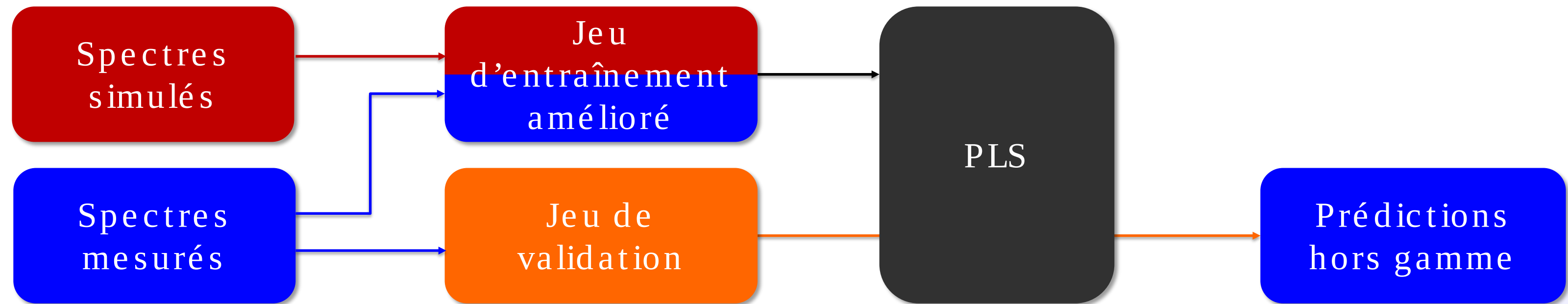
INRAE

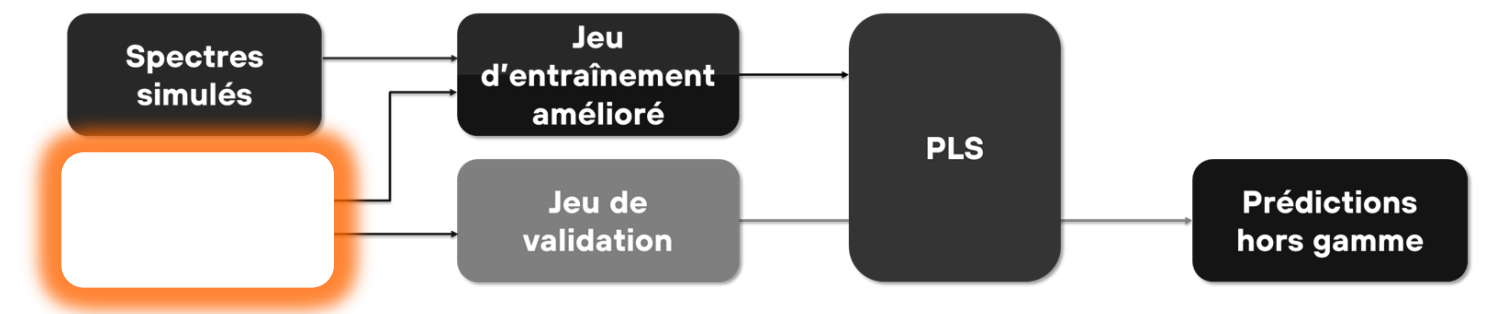
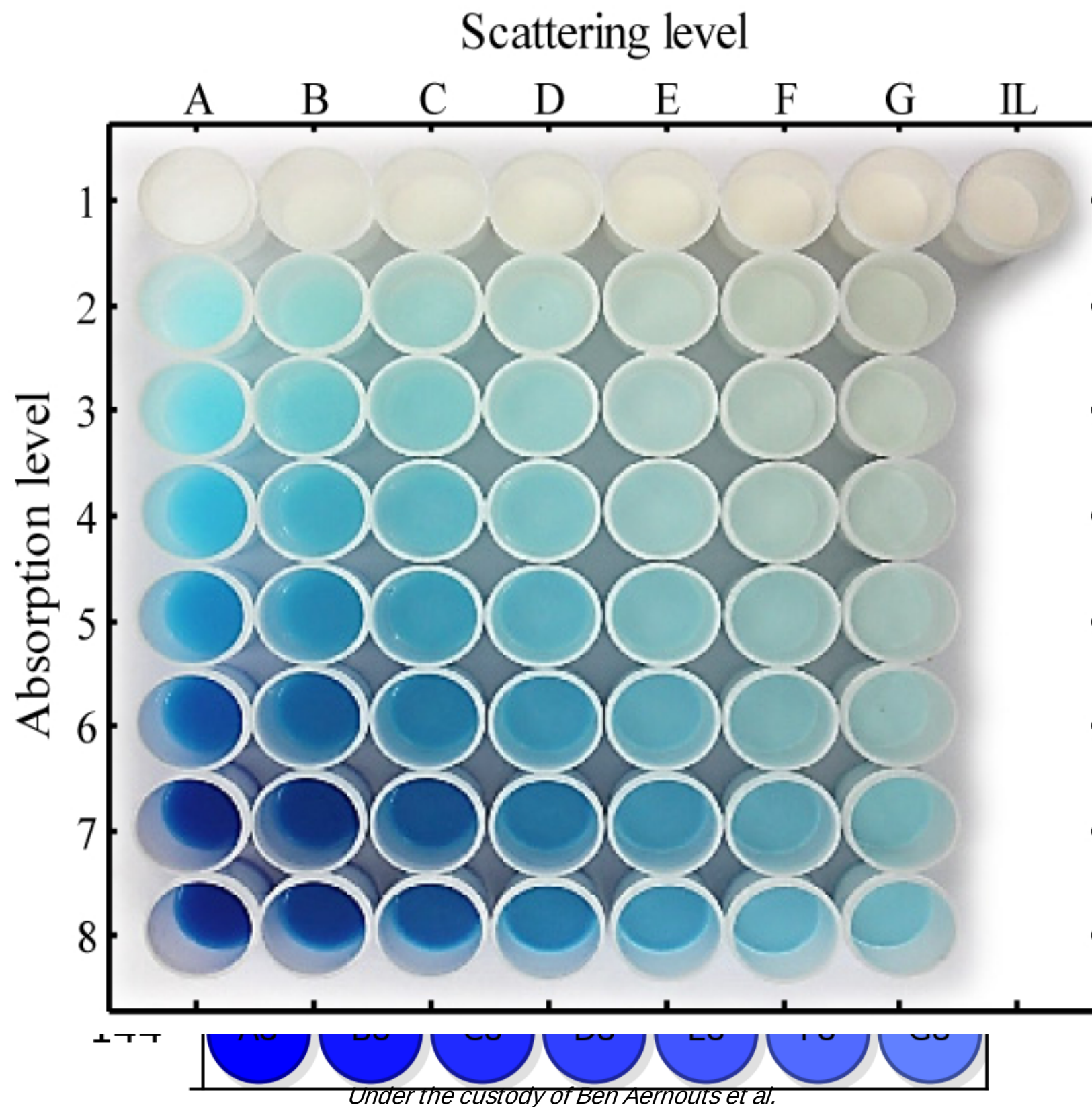
 CHAUVIN
ARNOUX
INDATECH

Déjà rêvé de prédire en dehors de la gamme de calibration?



Méthode proposée



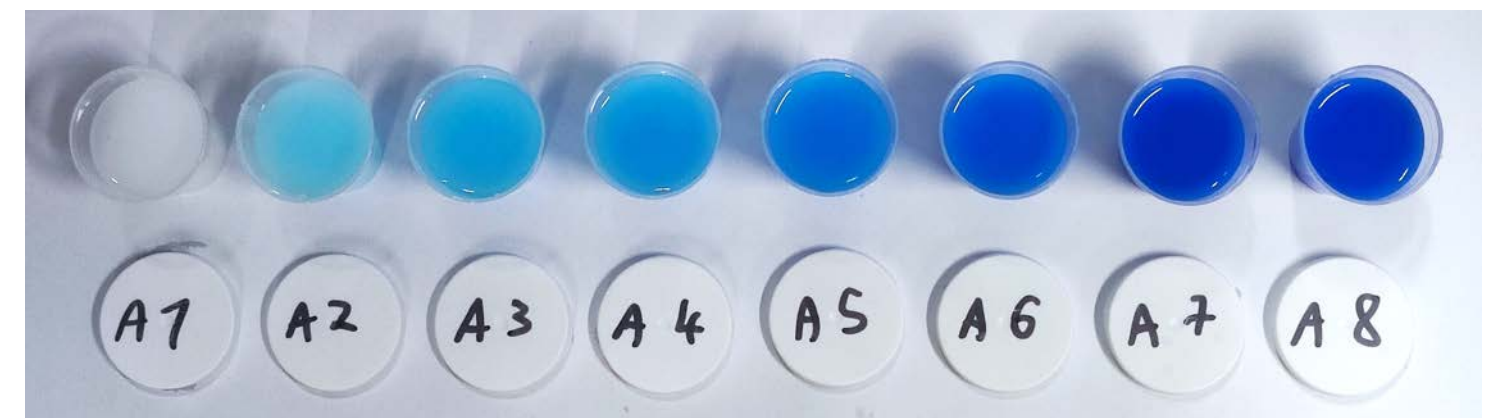


■ Fantômes liquides¹

Bleu de Méthylène (MB)

Intralipid® 20% (IL20%)

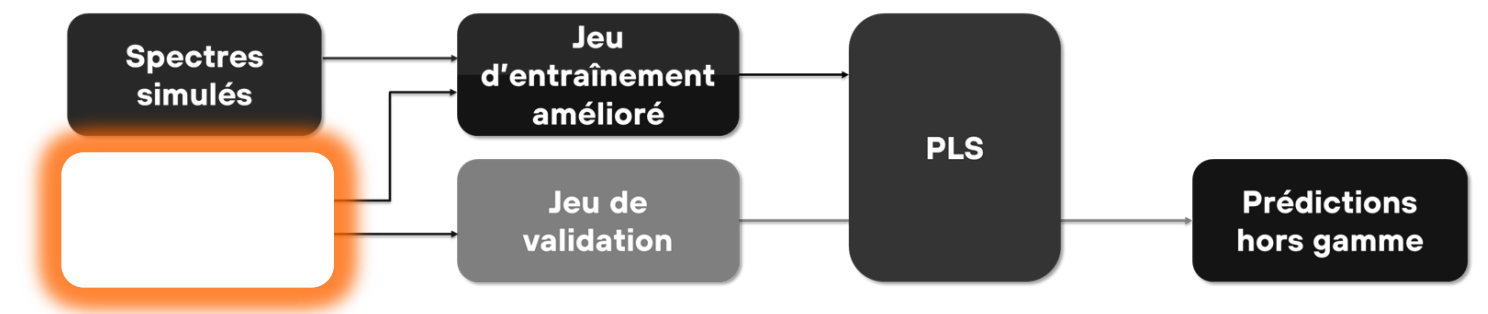
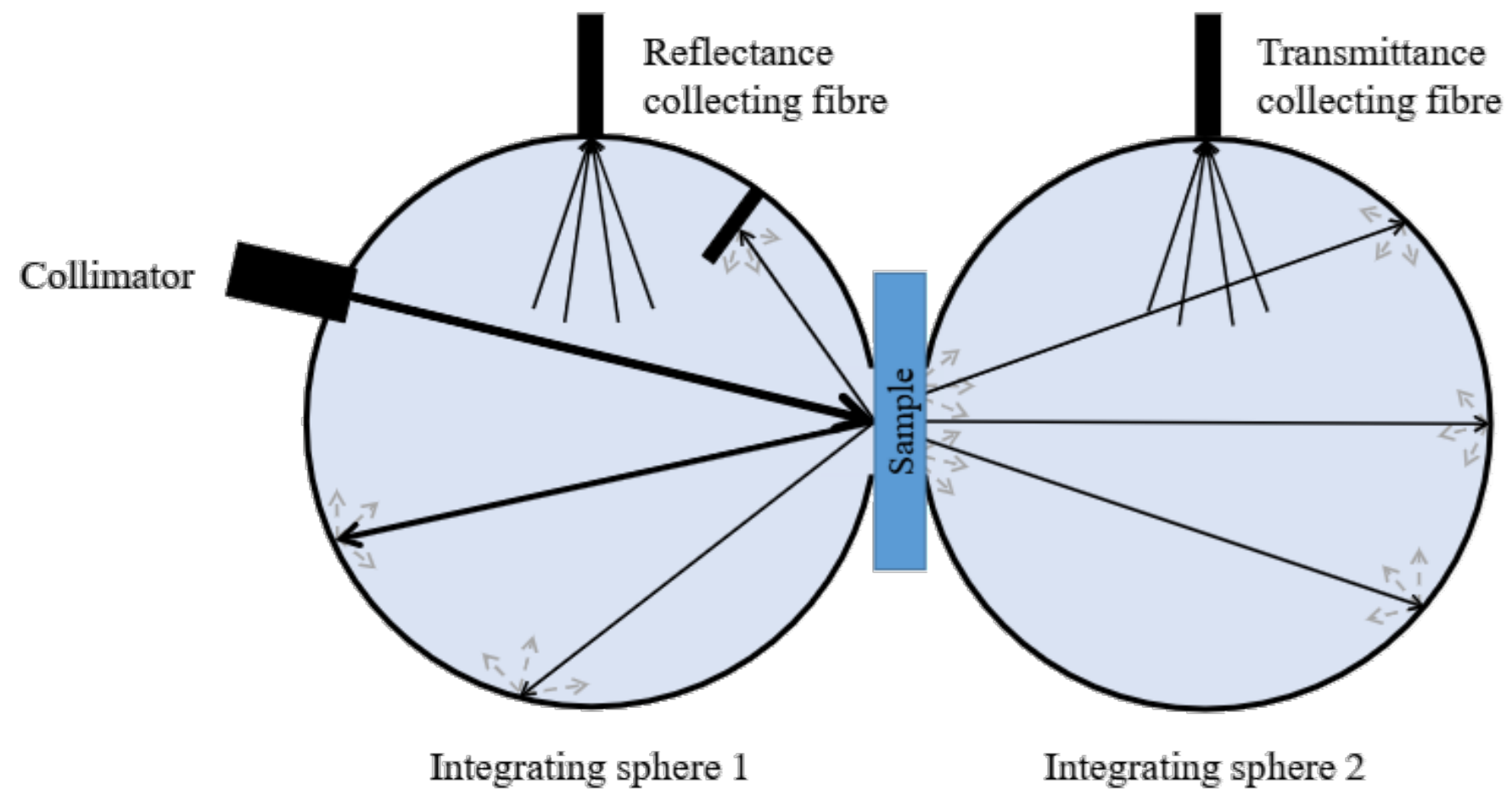
Eau



¹Aernouts Ben et al.

"Supercontinuum laser based optical characterization of Intralipid® phantoms in the 500-2250 nm range."

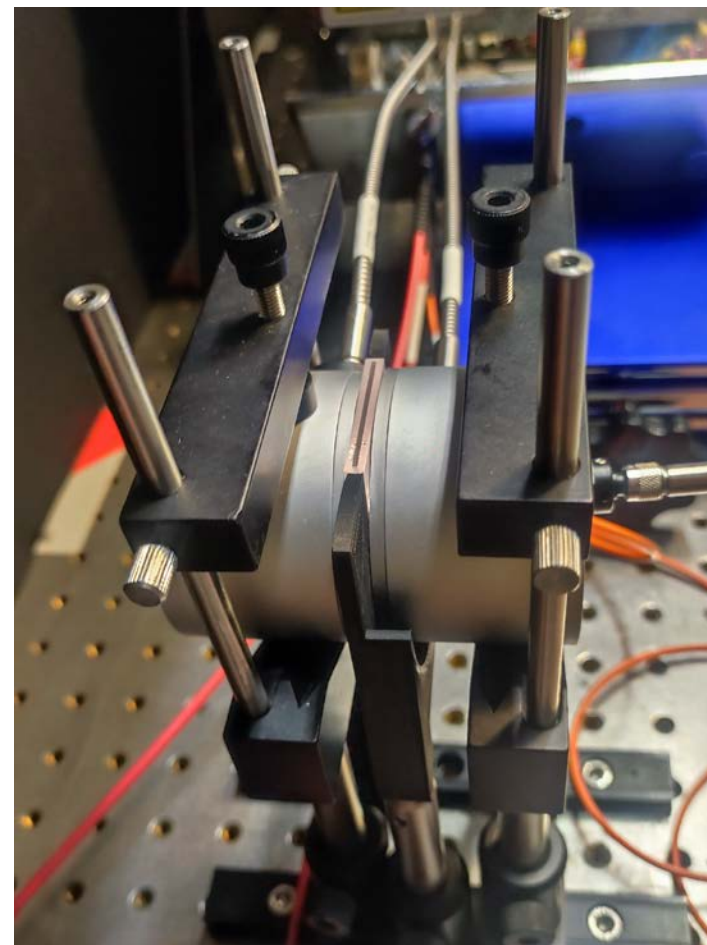
Optics express 2126 (2013): 32450-67.



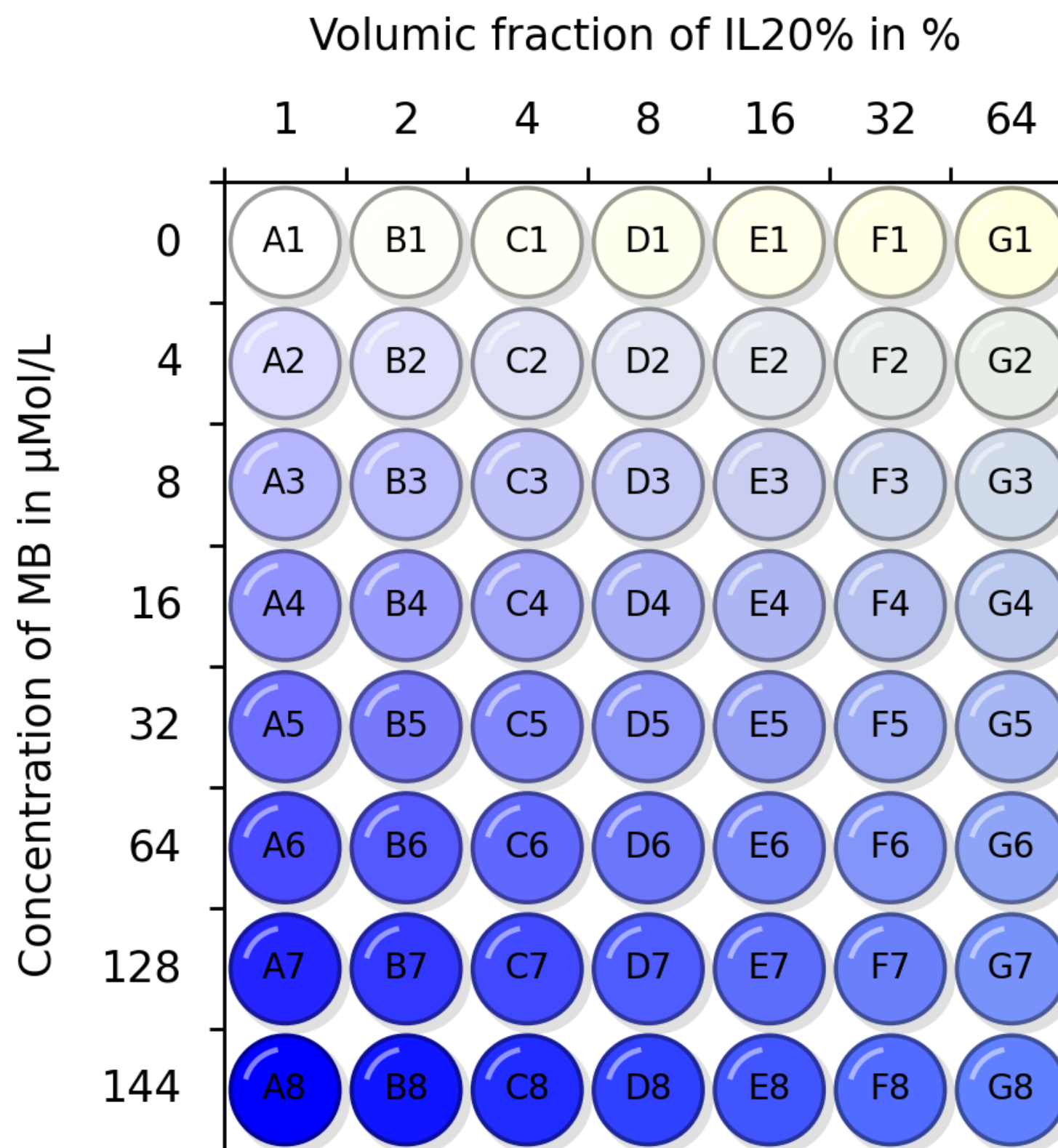
■ Double sphère d'intégration

2 spectromètres visible 400-800 nm

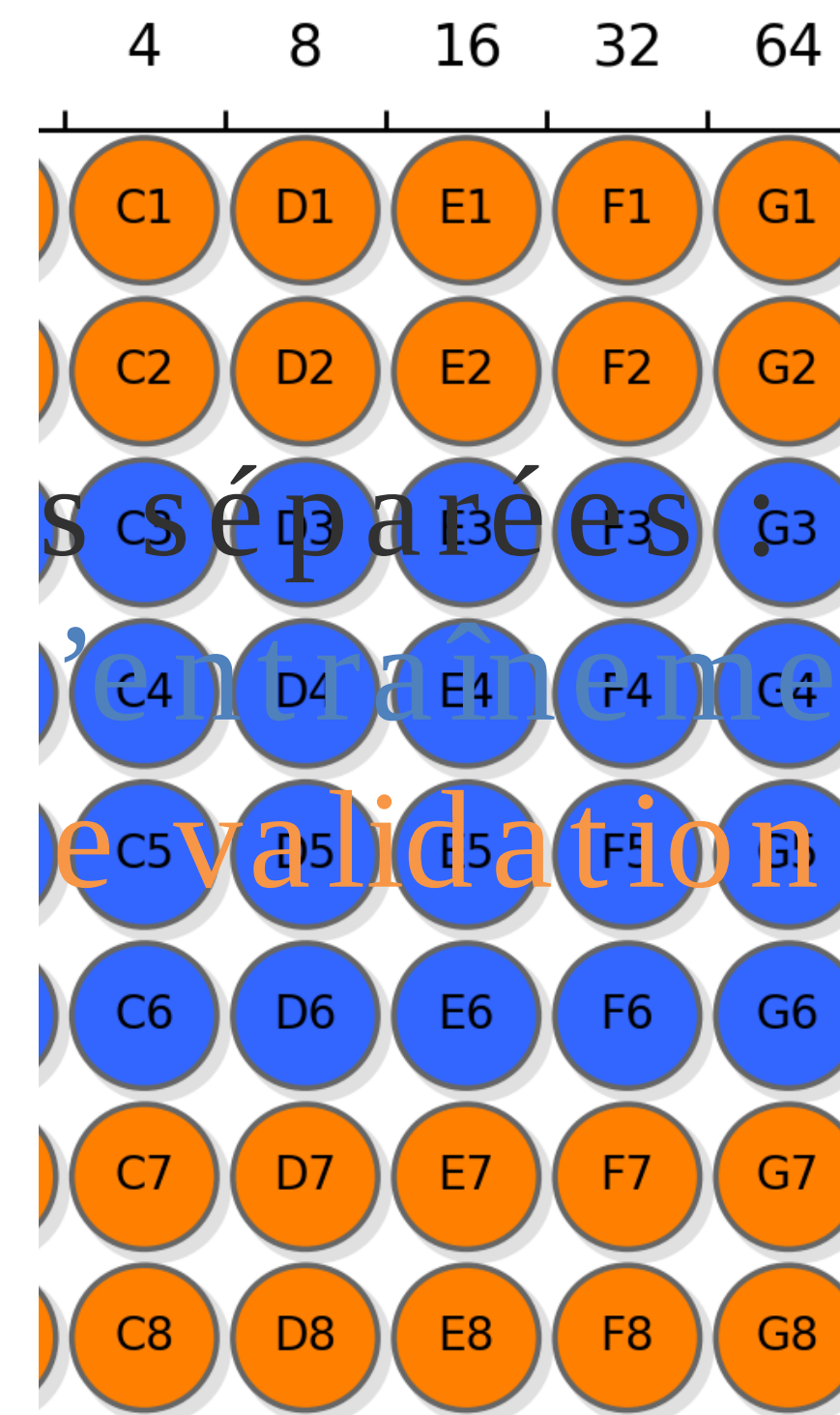
Cuvette 1mm



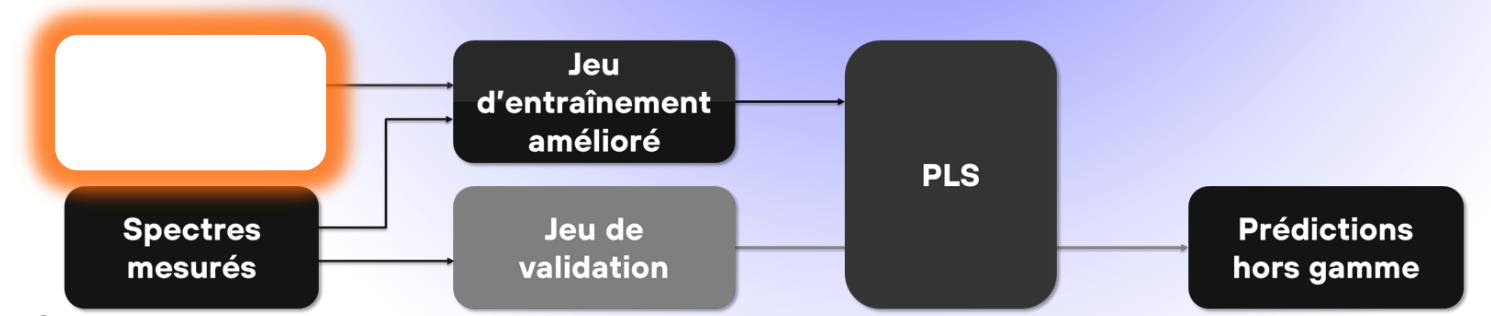
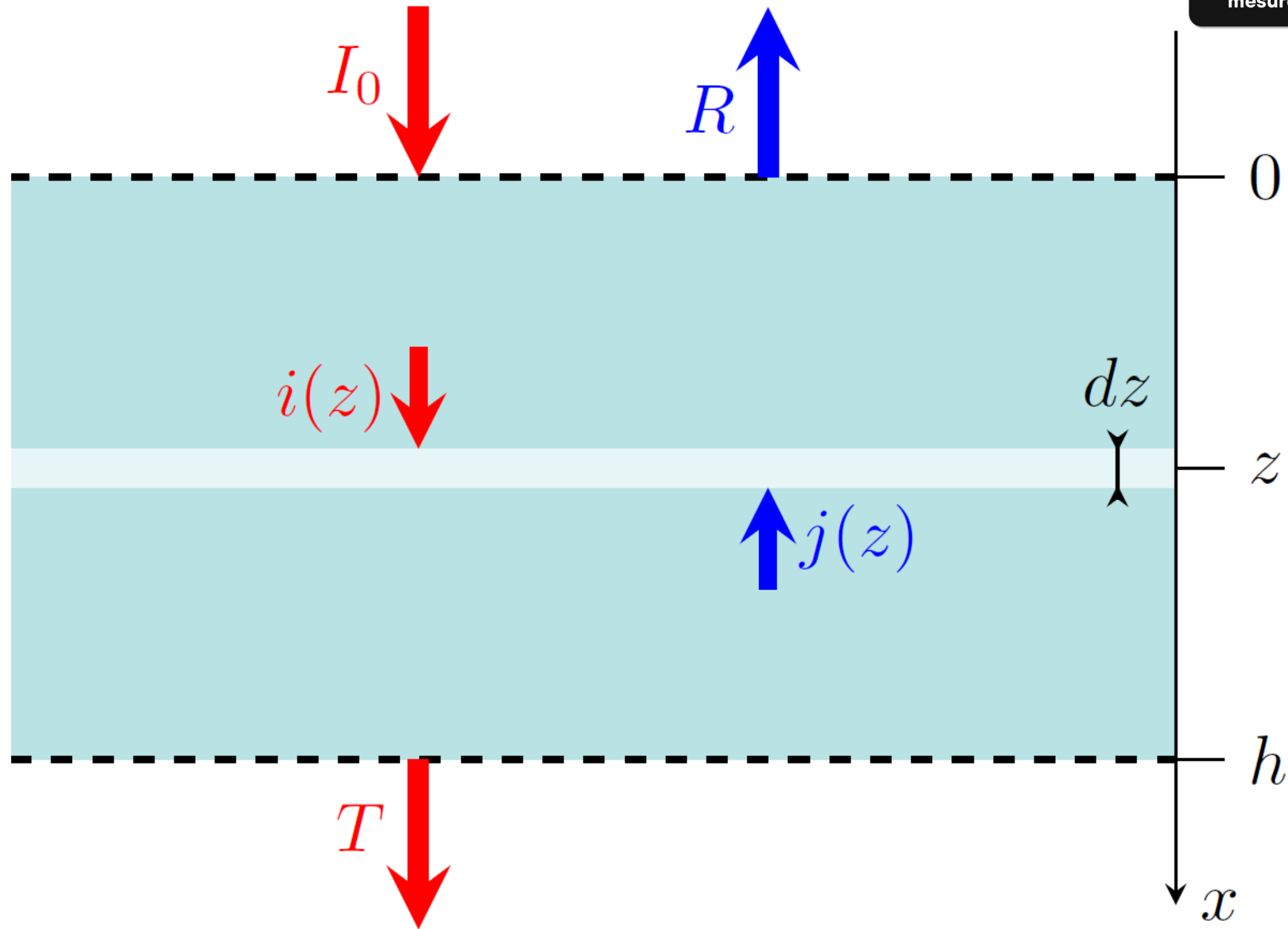
Cas A



Volumic fraction of IL20% in %



s séparées :
entraînement
évaluation



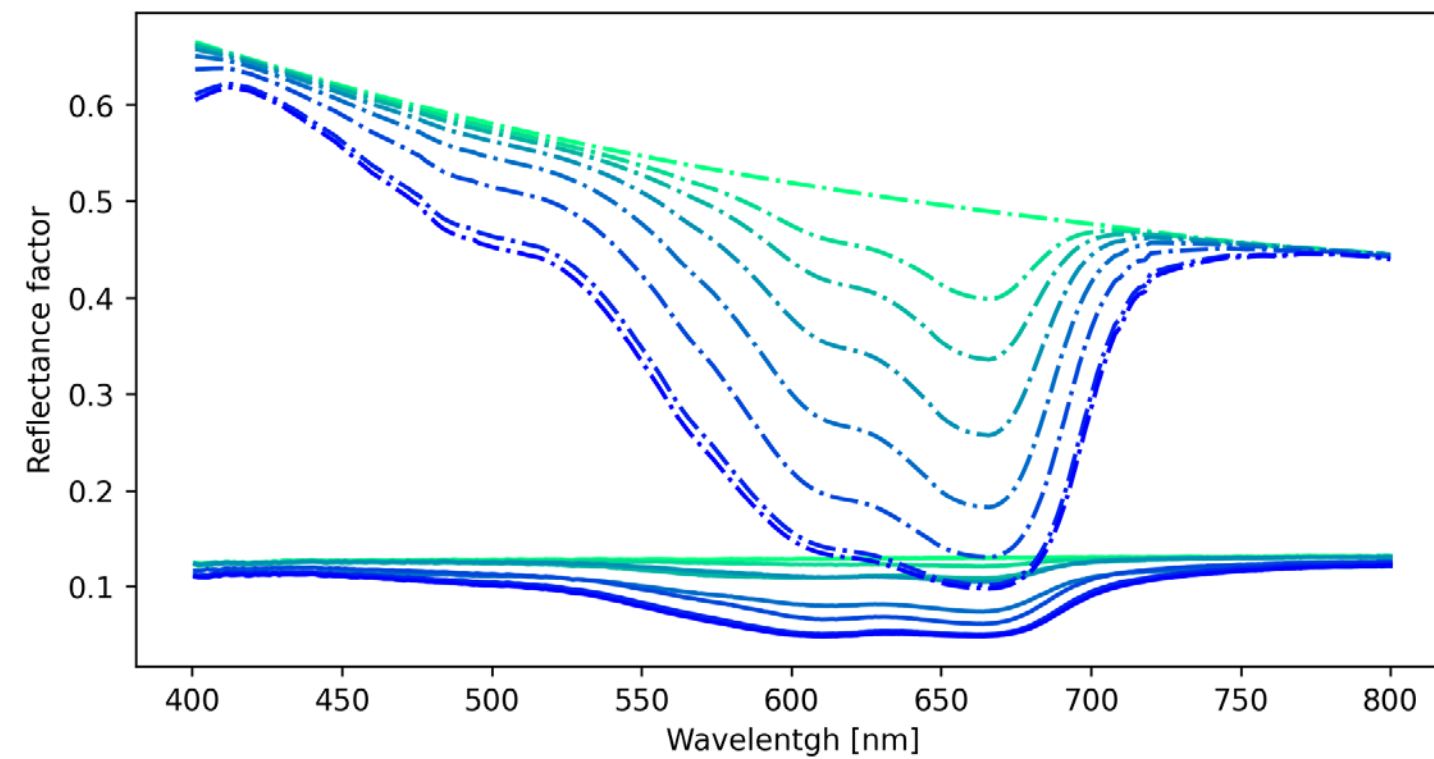
■ Kubelka-Munk¹ (2 flux)

Entrée : Bulk Optical Properties (μ_a , μ_s) des composes purs

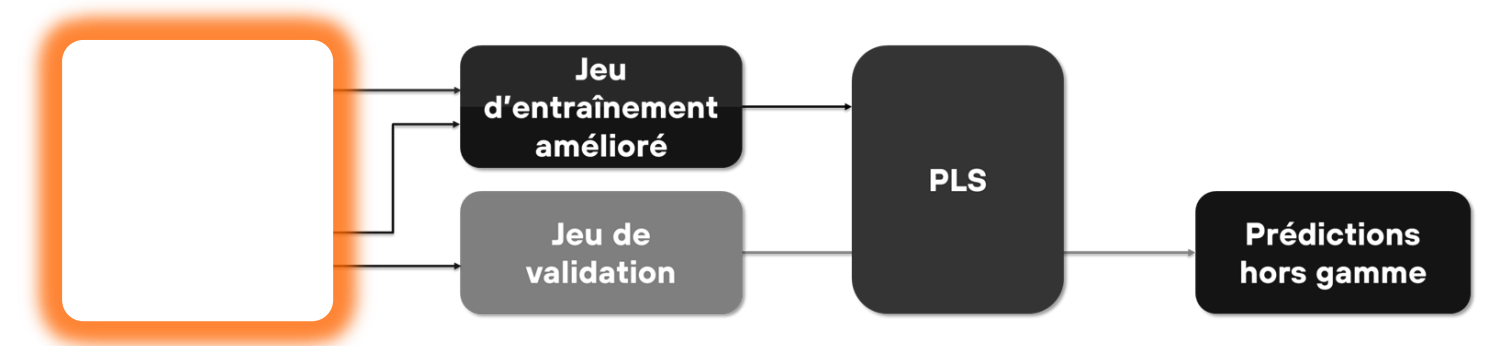
μ_a : absorption
 μ_s : diffusion

¹Kubelka, P., & Munk, F. (1931). An article on optics of paint layers. *Z. Tech. Phys.*, 12(593-601), 259-274.

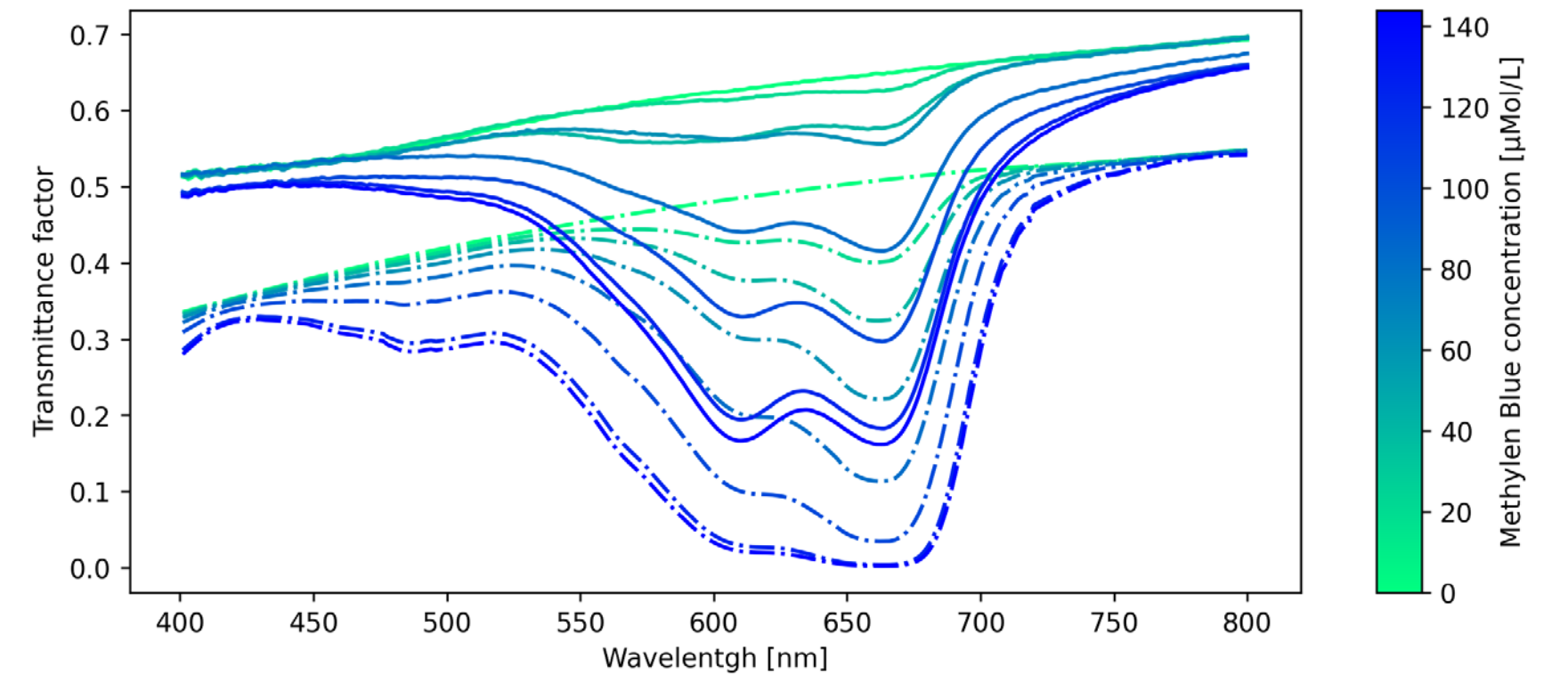
■ 1% Intralipids



■ Reflectance



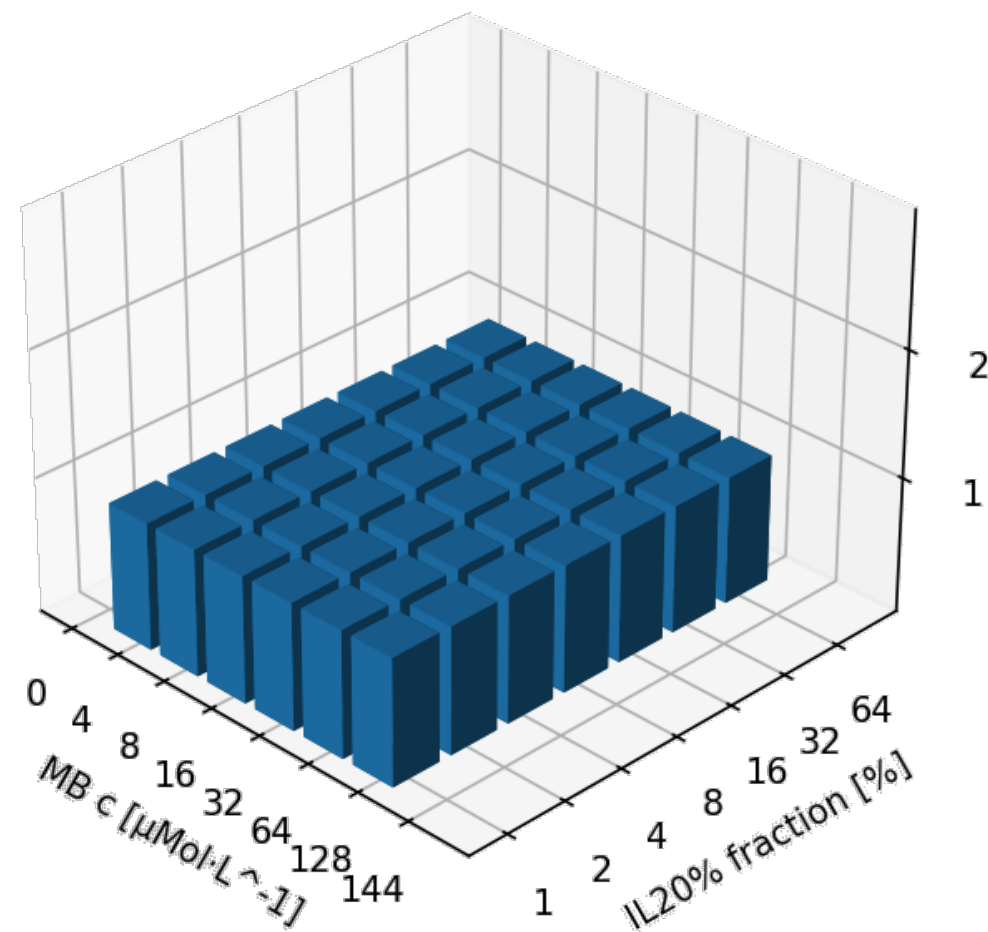
— Mesure
- - - Simulation



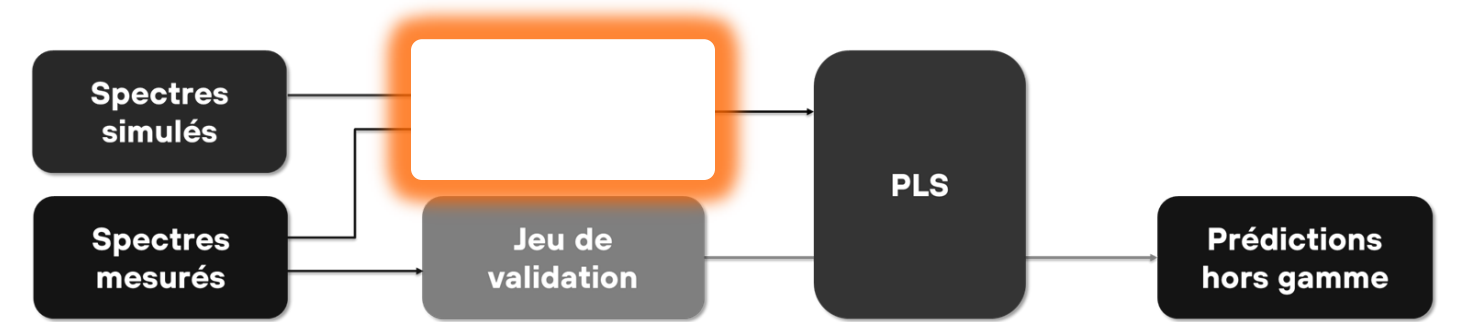
■ Transmittance

Cas A

- Spectres mesurés
- Spectres simulés



Reference



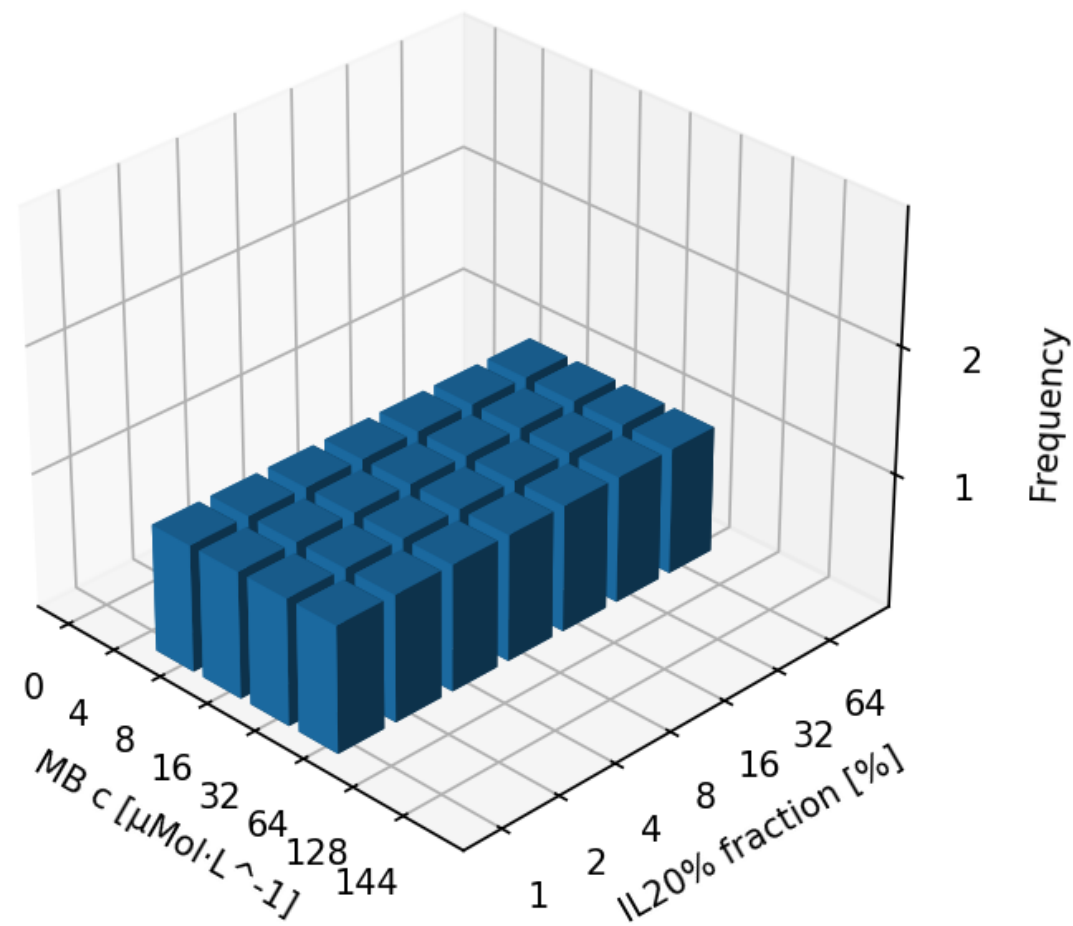
Complétion



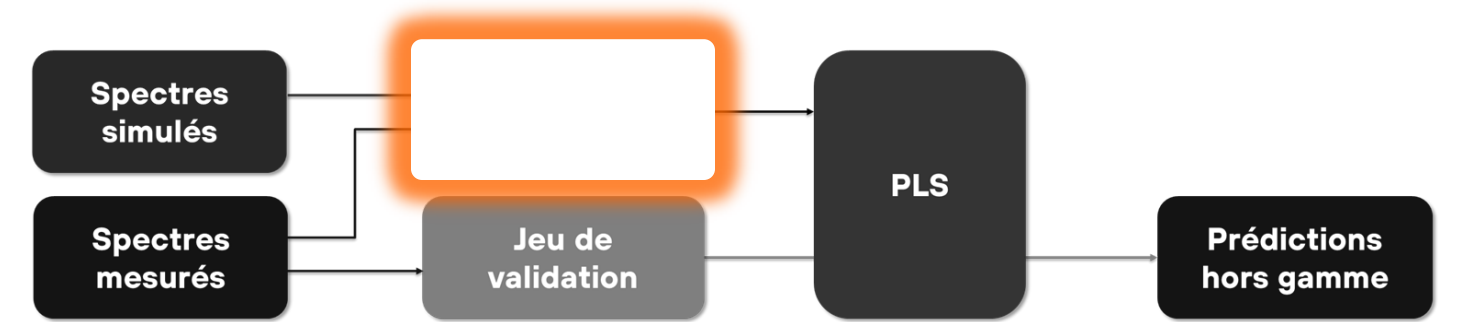
Superposition

Cas B

- Spectres mesurés
- Spectres simulés



Reference



Complétion



Superposition

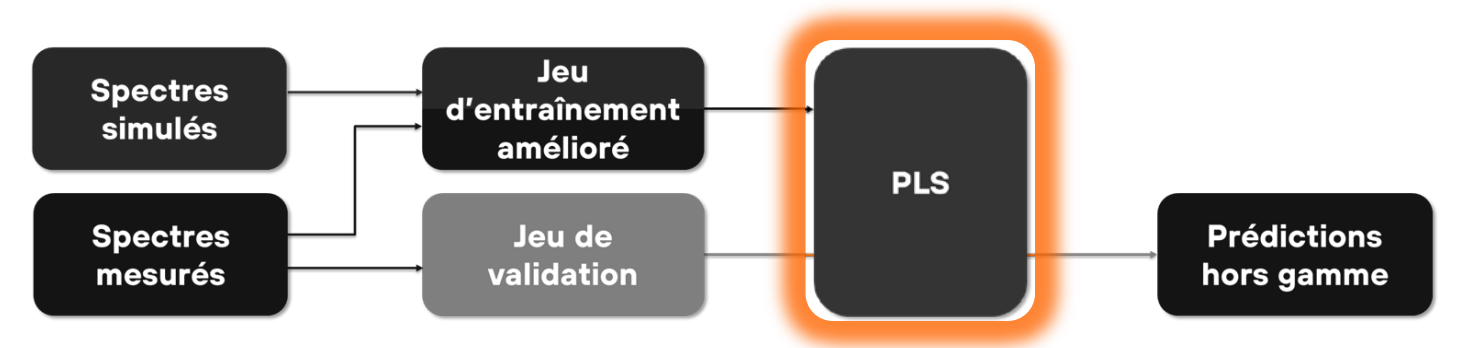
■ PLS sur la concentration en Bleu de Méthylène

Prétraitement

Standard Scaler

Jeux d'entraînement

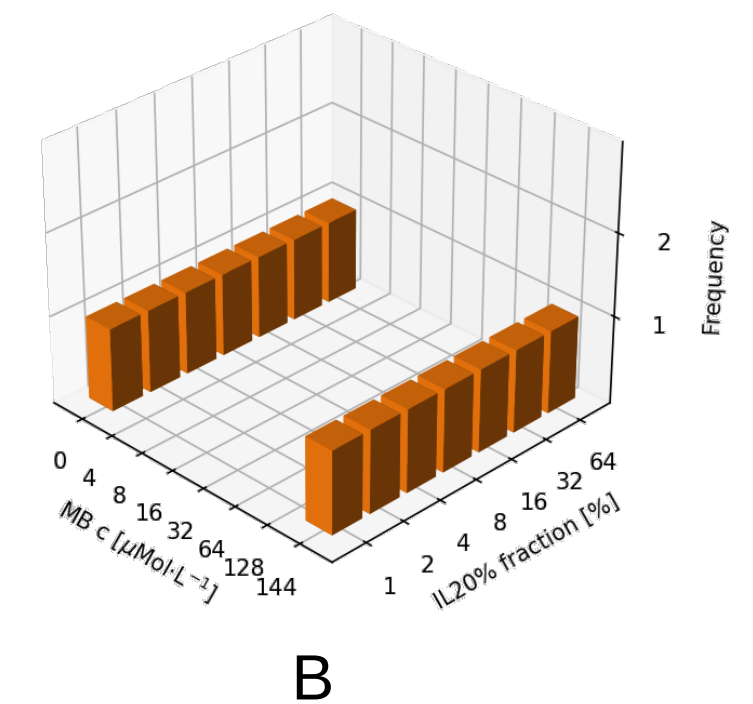
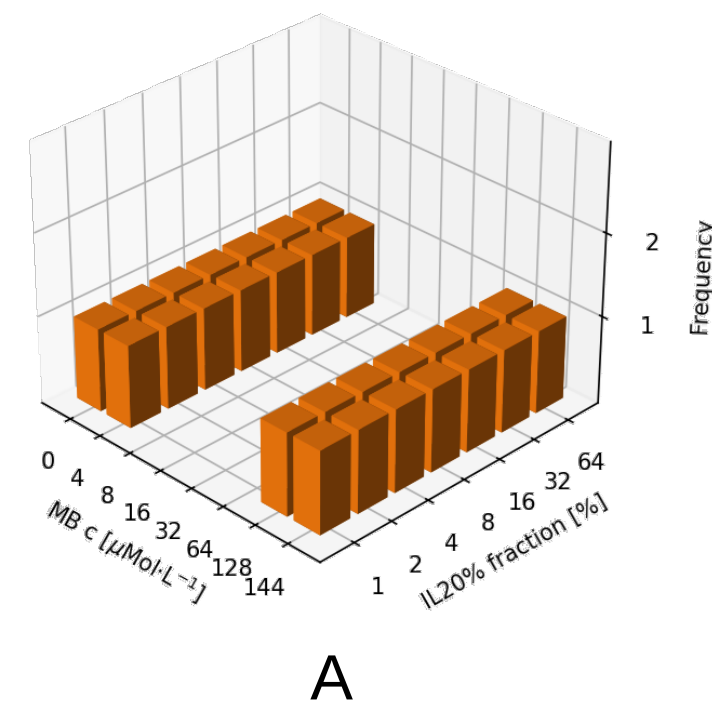
Cas	Mode	Méthode
A	R	Référence
B	T	Complétion
Concaténés		Superposition



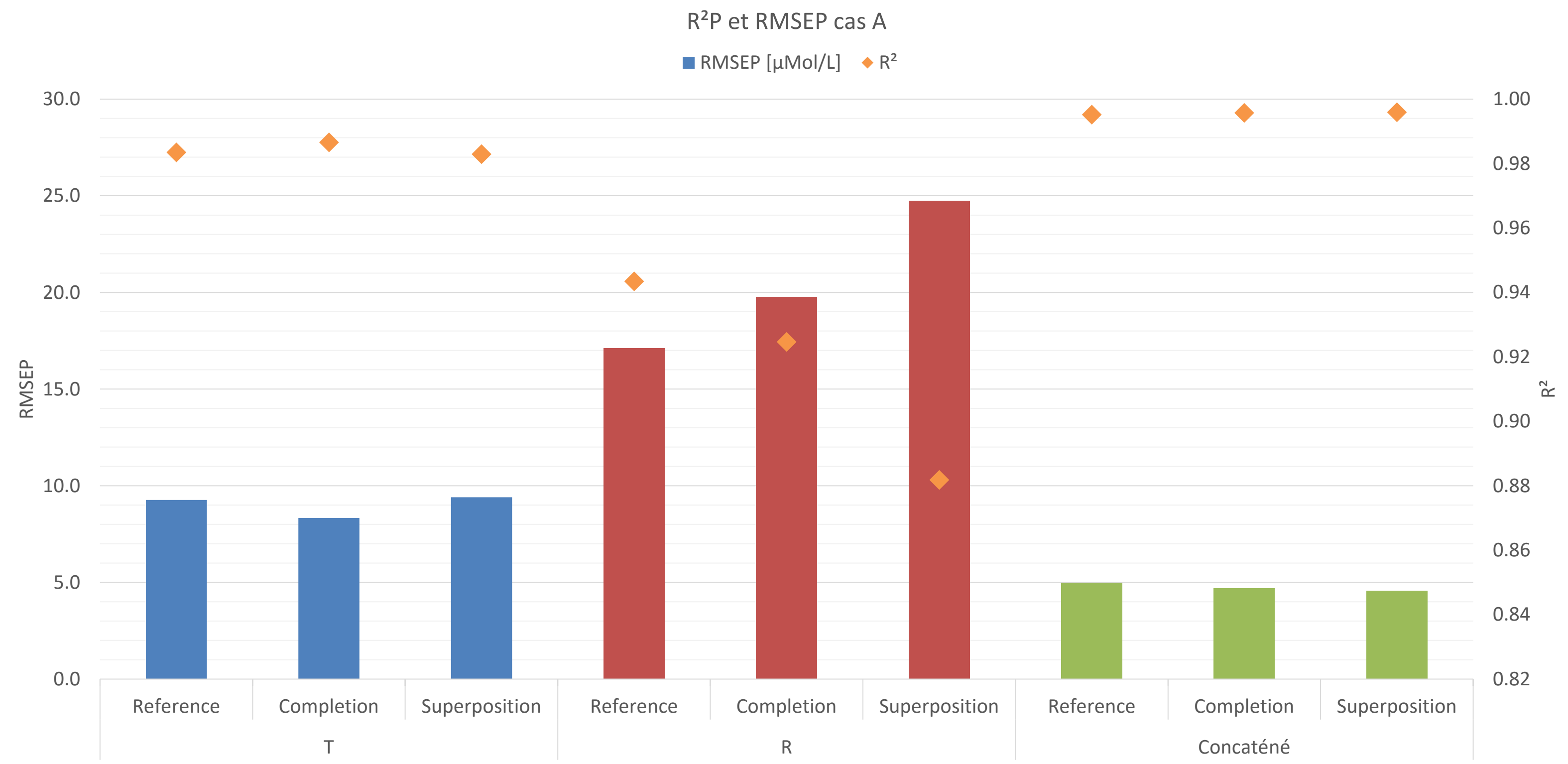
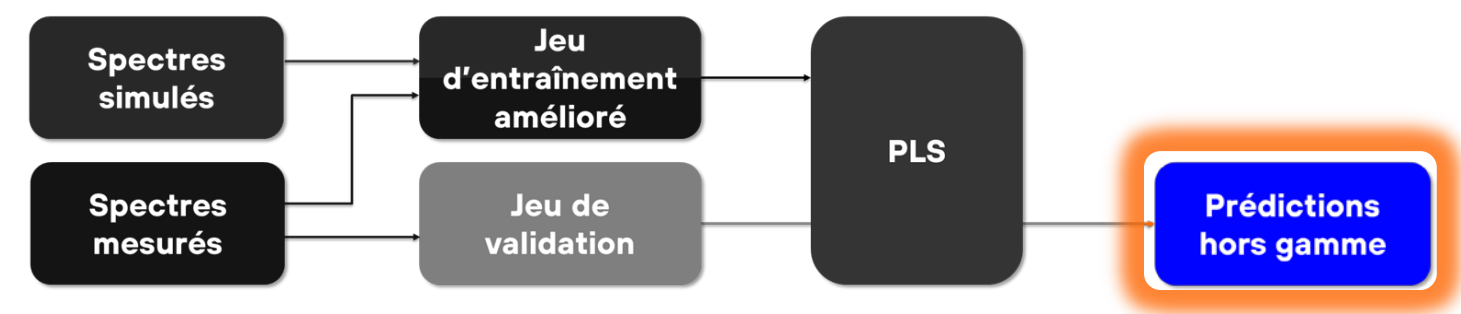
Cross-validation

8 Folds 20 répétitions

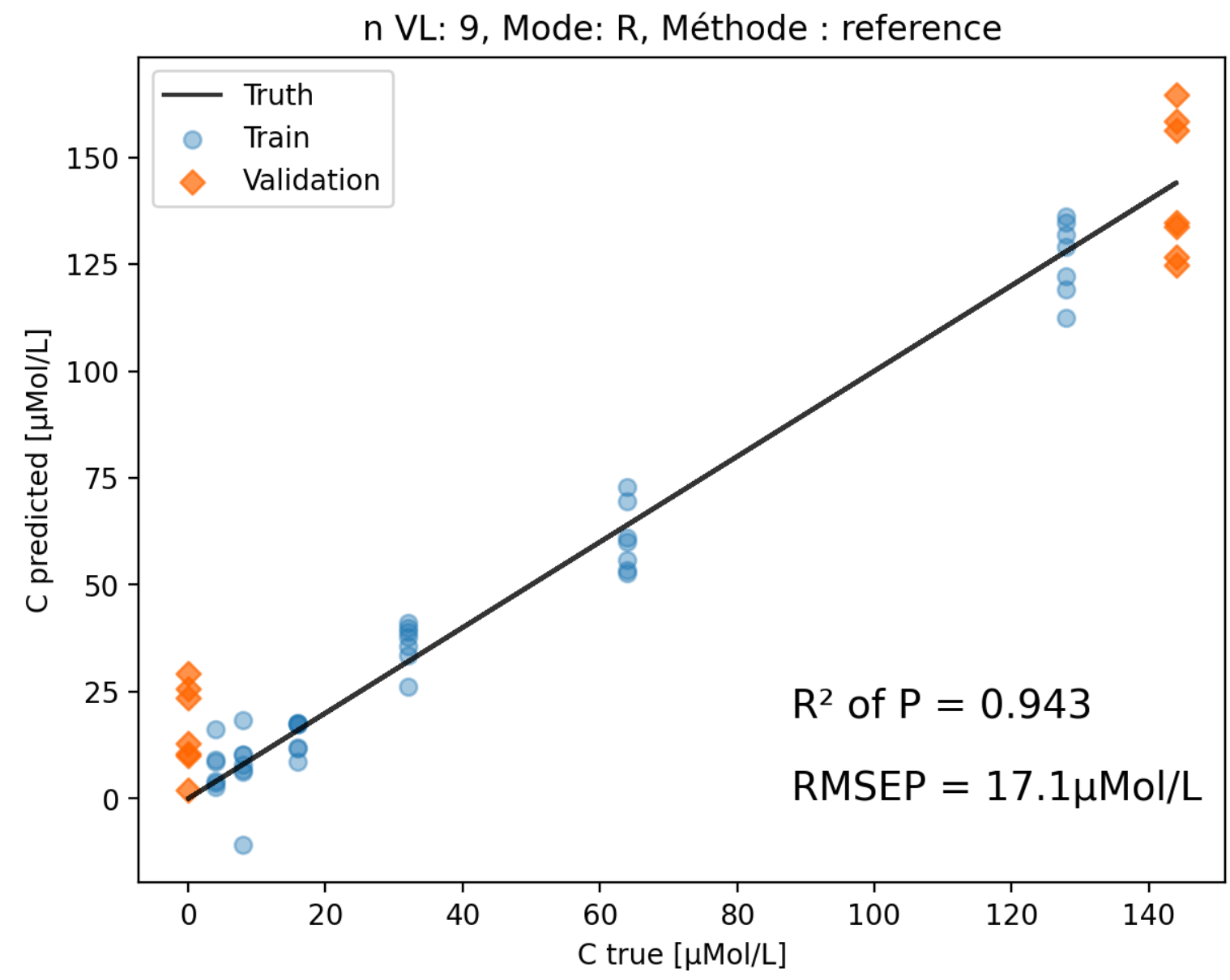
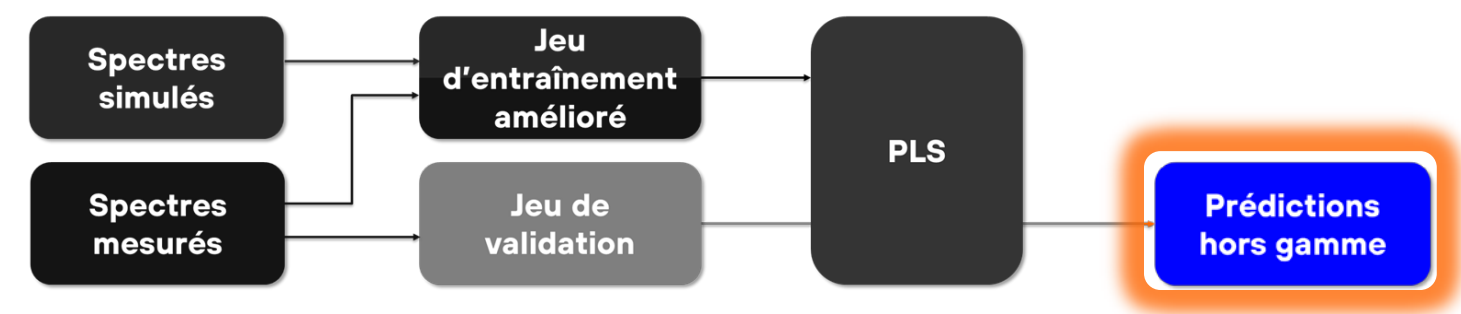
Jeux de validation



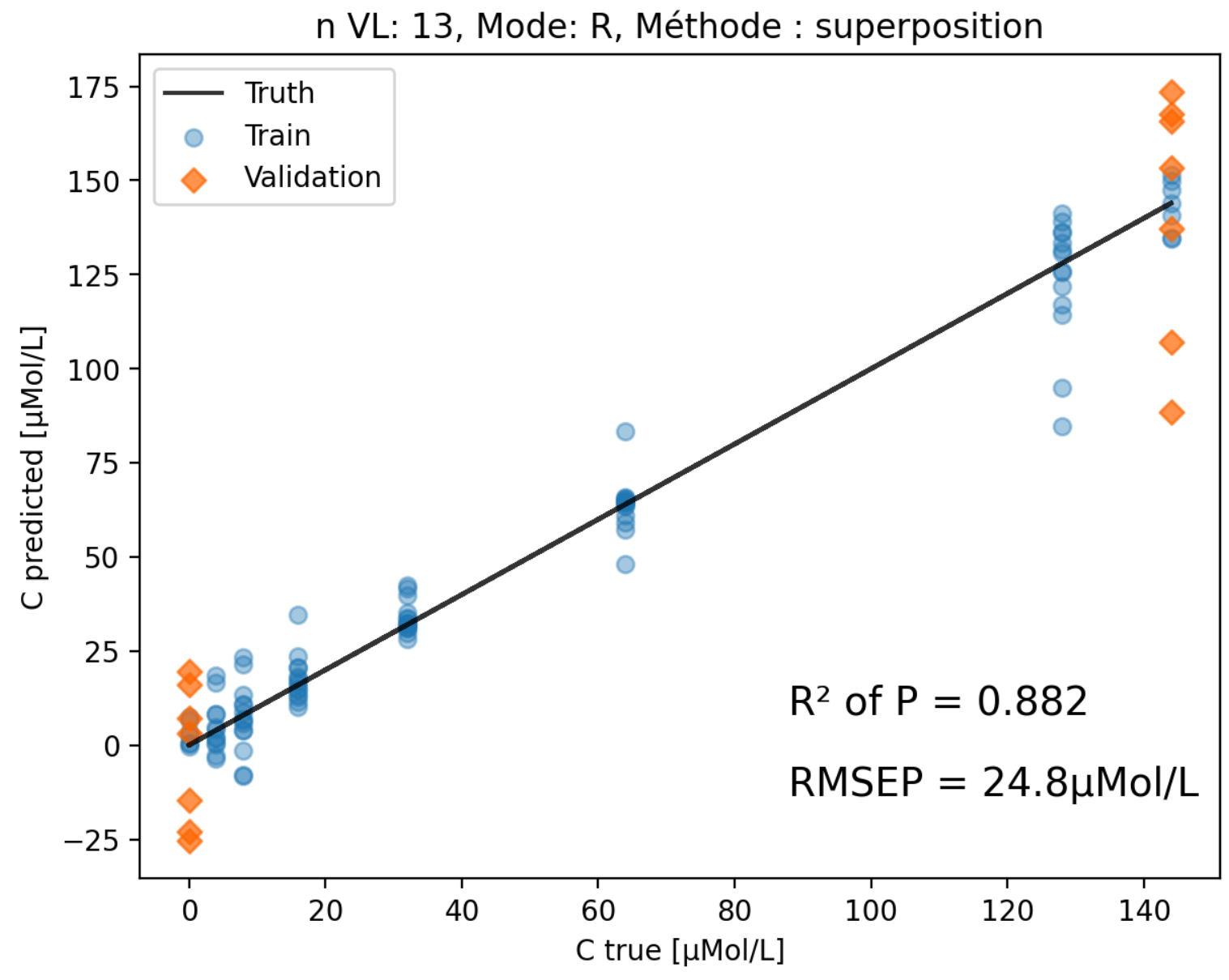
Cas A



Cas A Reflectance

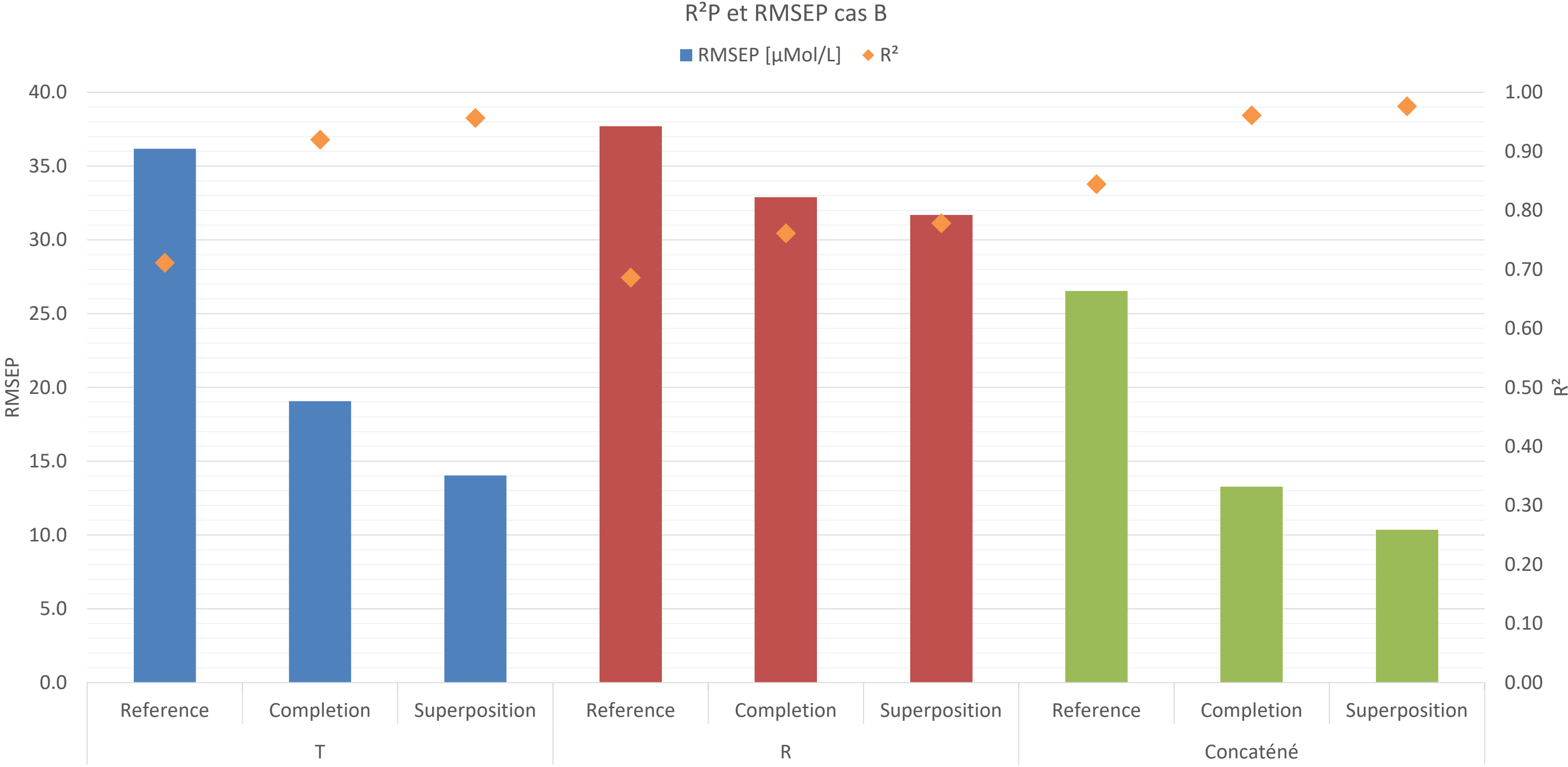
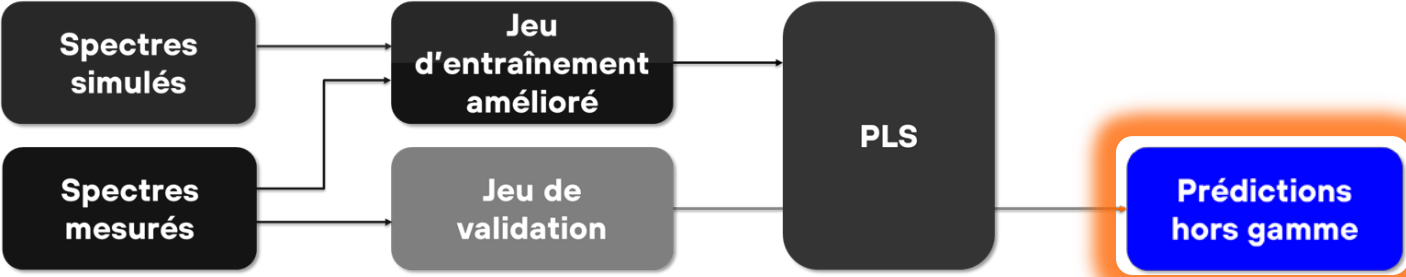


Référence

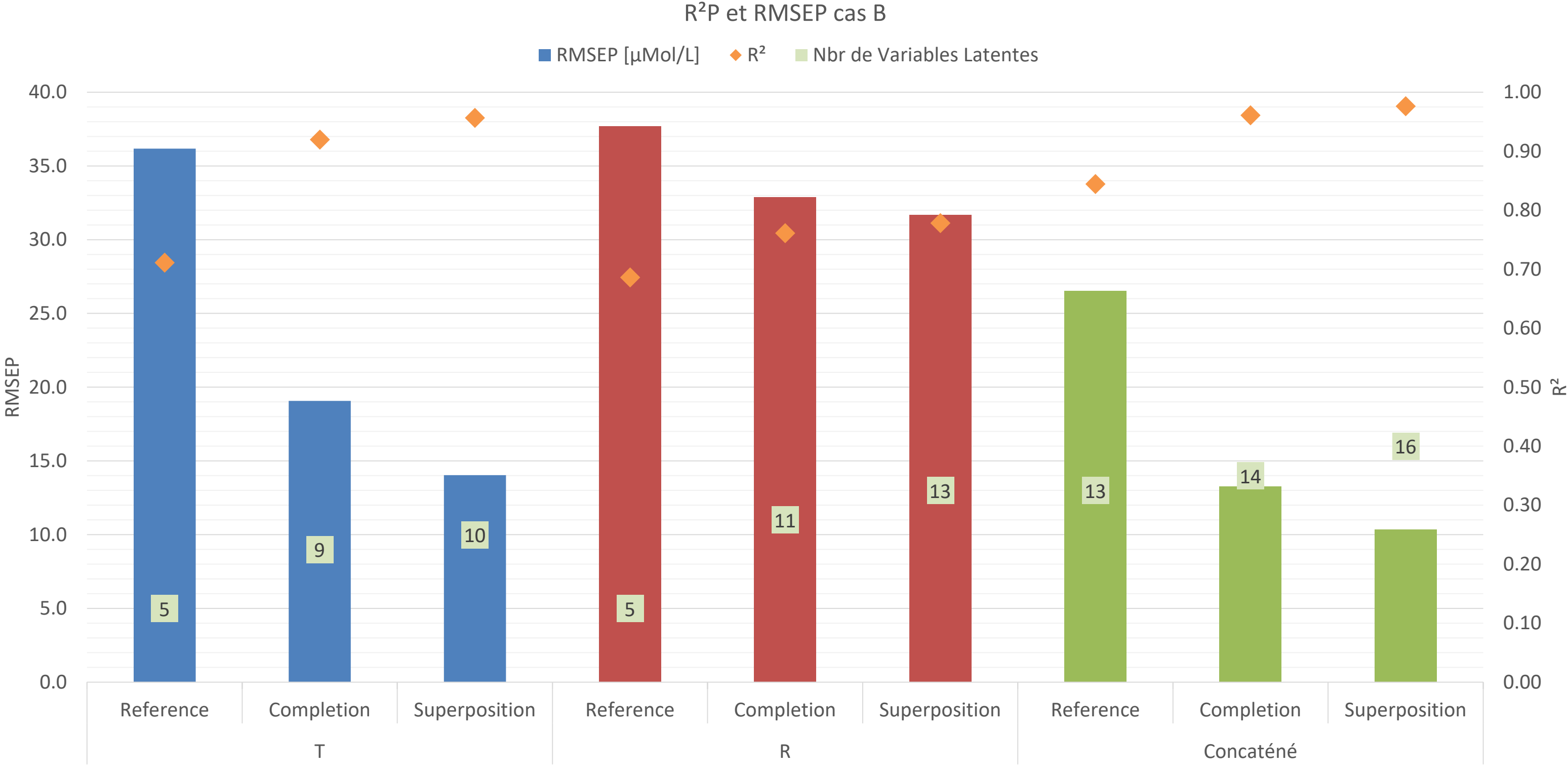
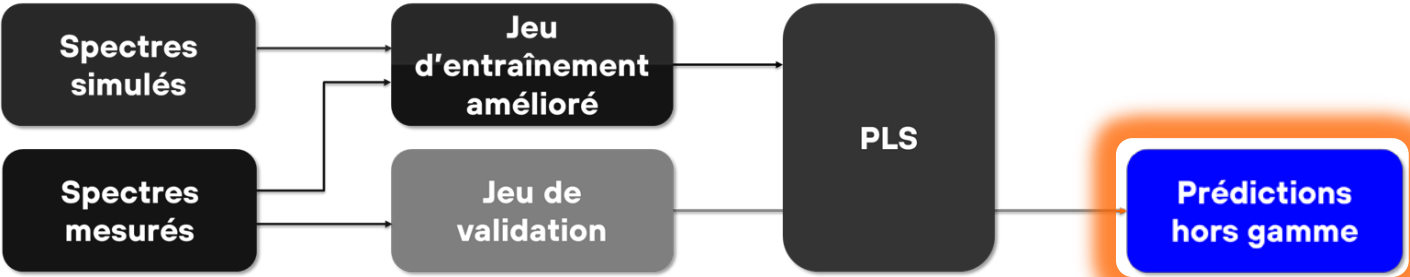


Superposition

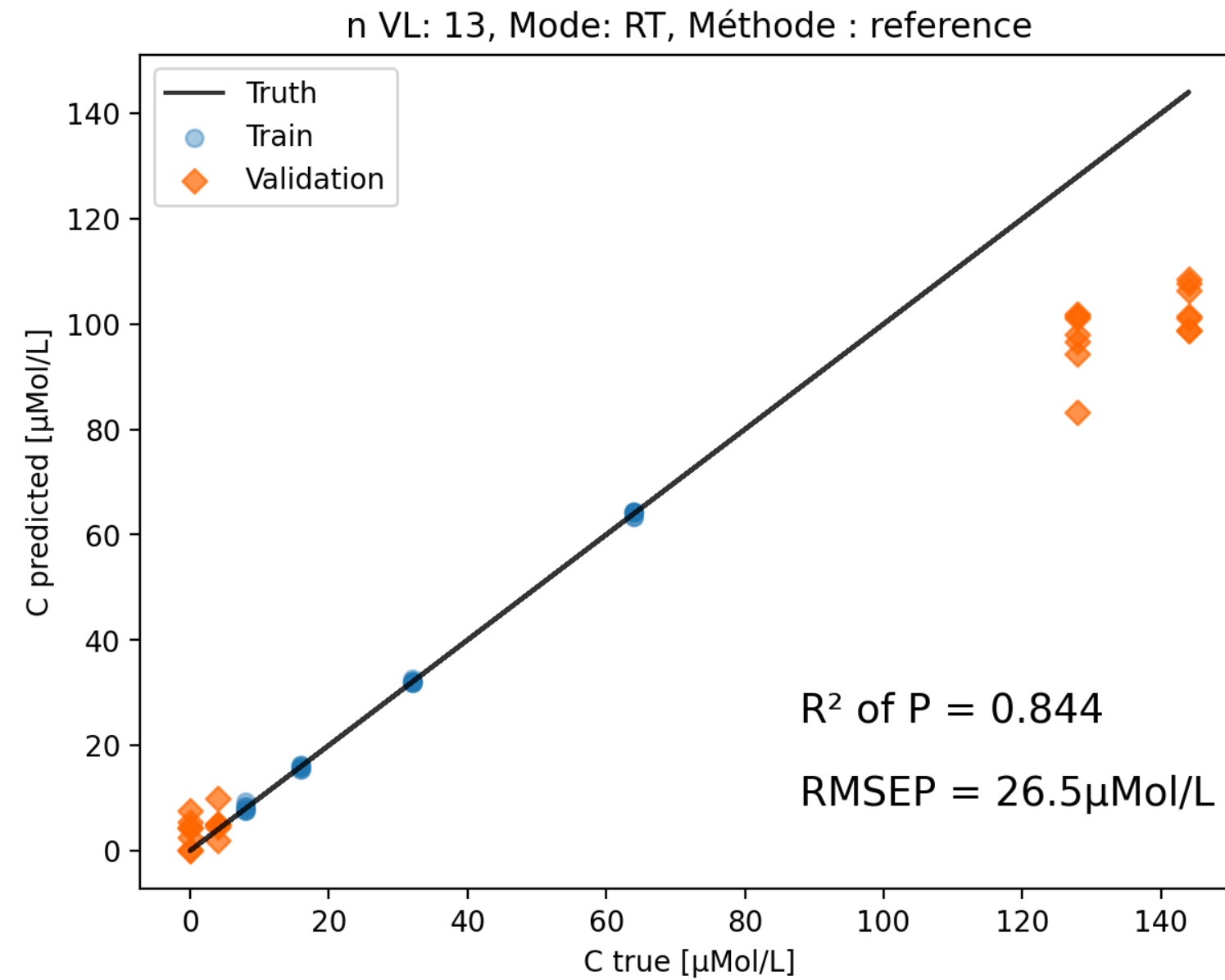
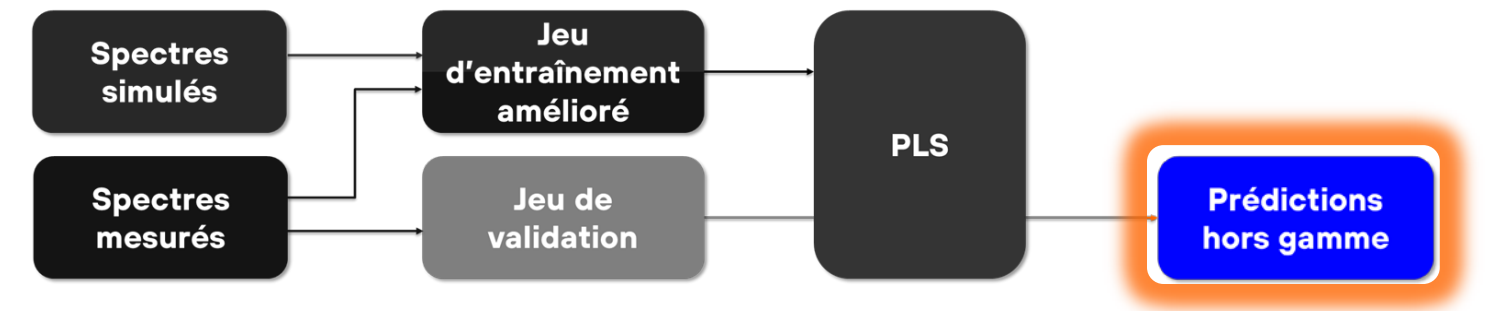
Cas B



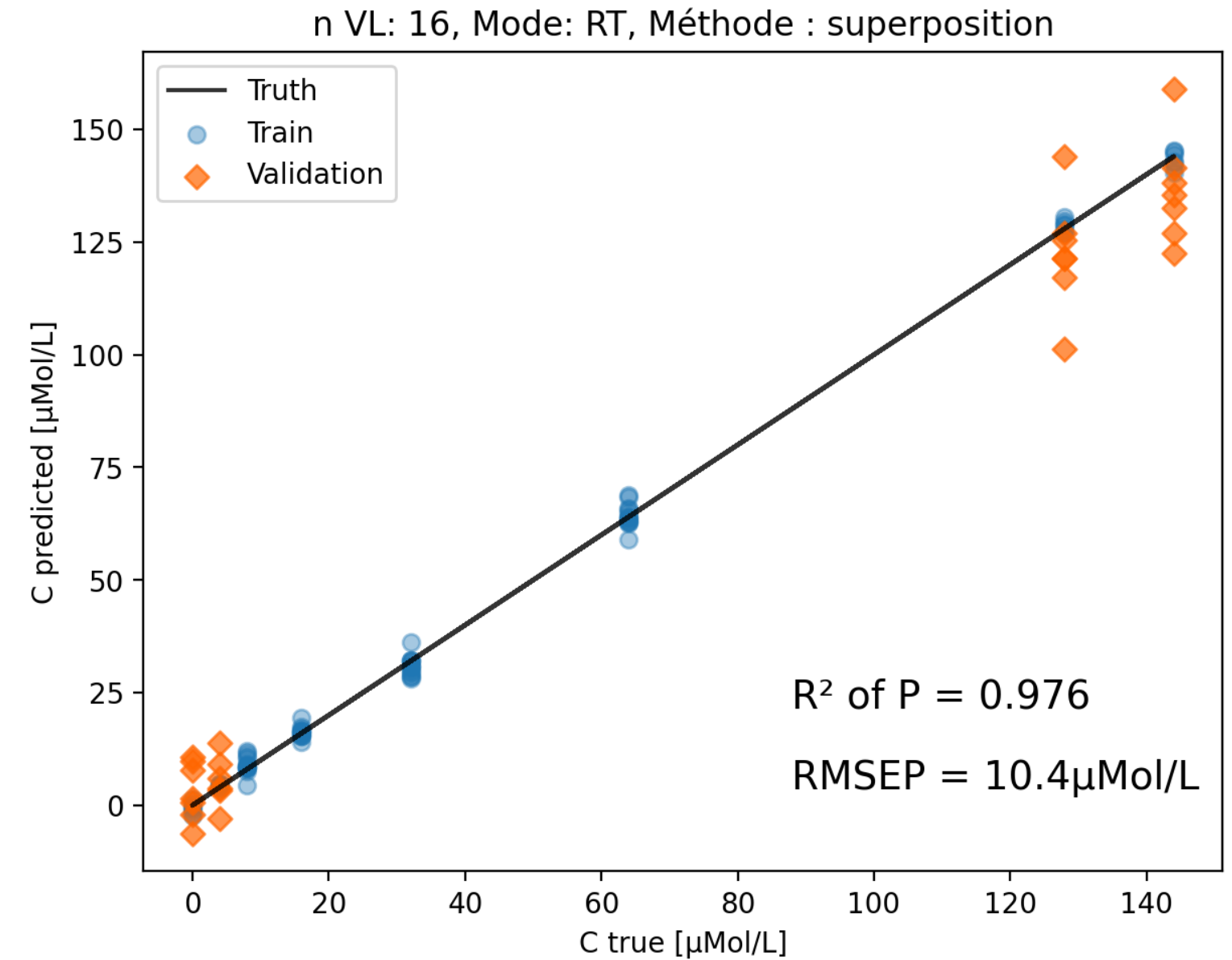
Cas B



Cas B Concaténés



Référence



Superposition

Conclusions & Perspectives

1 Une méthode simple permet de prédire en dehors de la gamme de calibration.

2 Applications potentielles pour tous les domaines utilisant la spectroscopie

3 Work in progress:
– Monte Carlo
– SRS
– Méthode différente

4 Perspectives
– NIR
– Deep learning

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