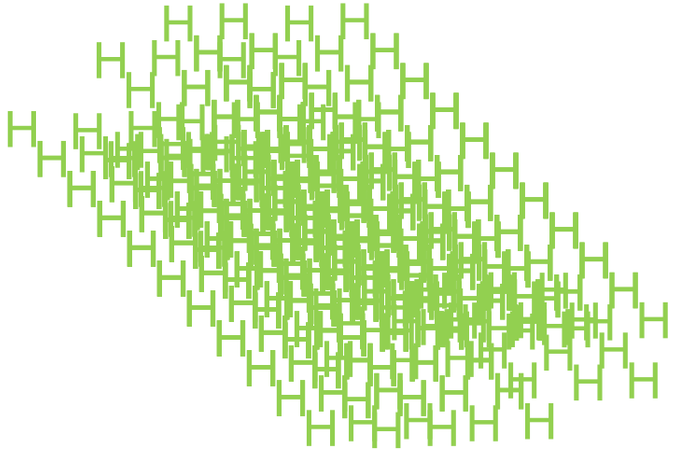
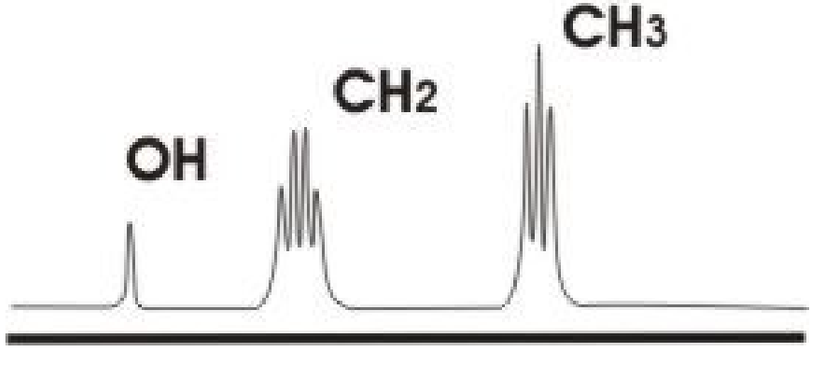
Start Part B

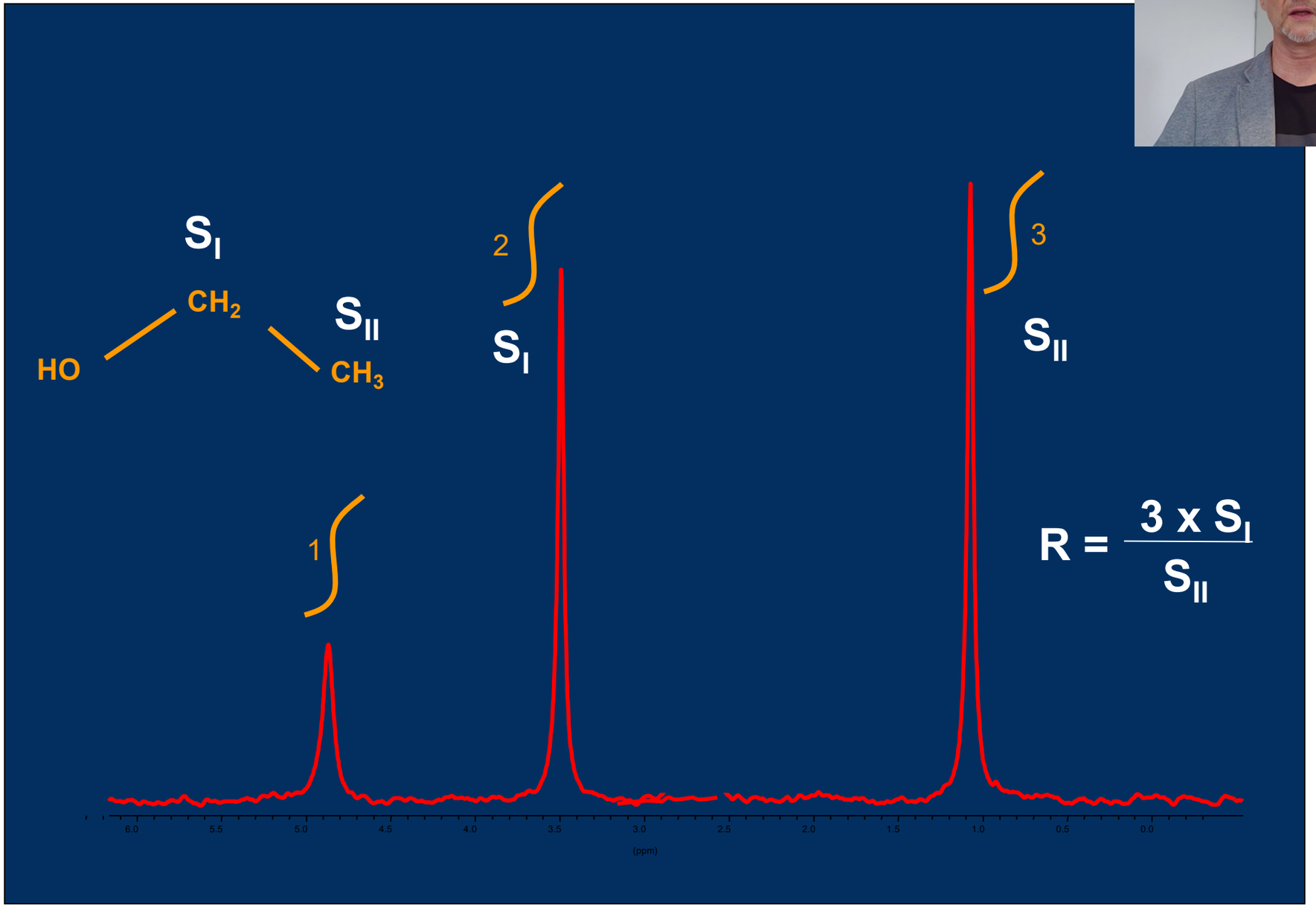
Thought Experiment

Statistical distribution of deuterium

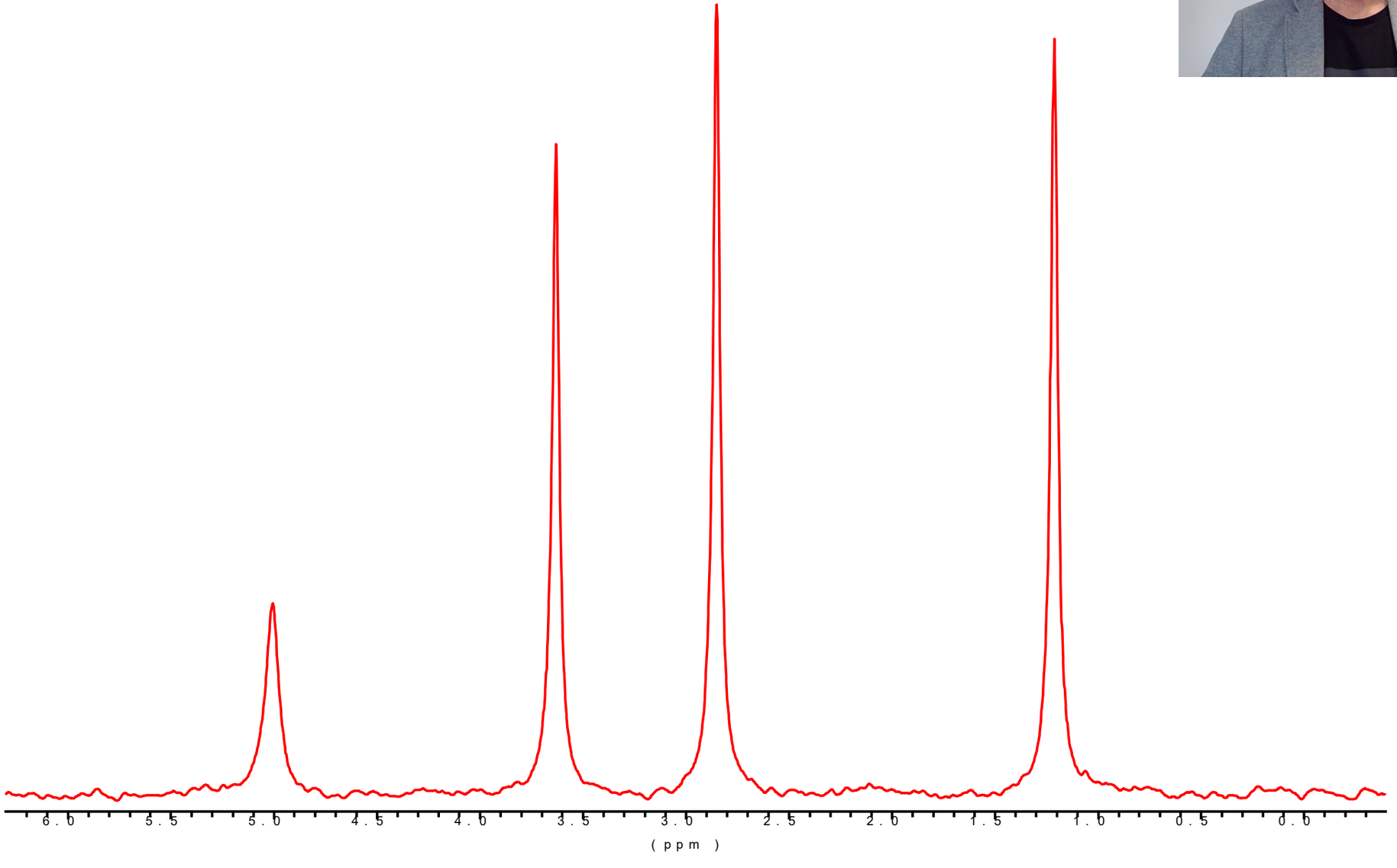




SNIF-NMR® (^{2}H-NMR)



SNIF-NMR® (^{2}H-NMR)



Calculations

$$(D/H)_i^A = \frac{P^{ST}}{P_i^A} \times \frac{M^A}{M^{ST}} \times \frac{m^{ST}}{m^A} \times \frac{{}^2H I_i^A}{{}^2H I^{ST}} \times (D/H)^{ST}$$

$(D/H)_i$	Site-specific isotope ratio
P	Number of equivalent positions of hydrogen atoms
M	Molecular weight
m	Mass
${}^{2H}I$	Signal intensity of ^{2}H
ST	Standard
A	Sample A

Martin et al., *Tetrahedron* **41**, 32

Wine Authentication

- determination of **deuterium distribution** in wine ethanol by **SNIF-NMR spectroscopy** (OIV MA-AS311-05):

wine sample

sample preparation (extraction of ethanol)

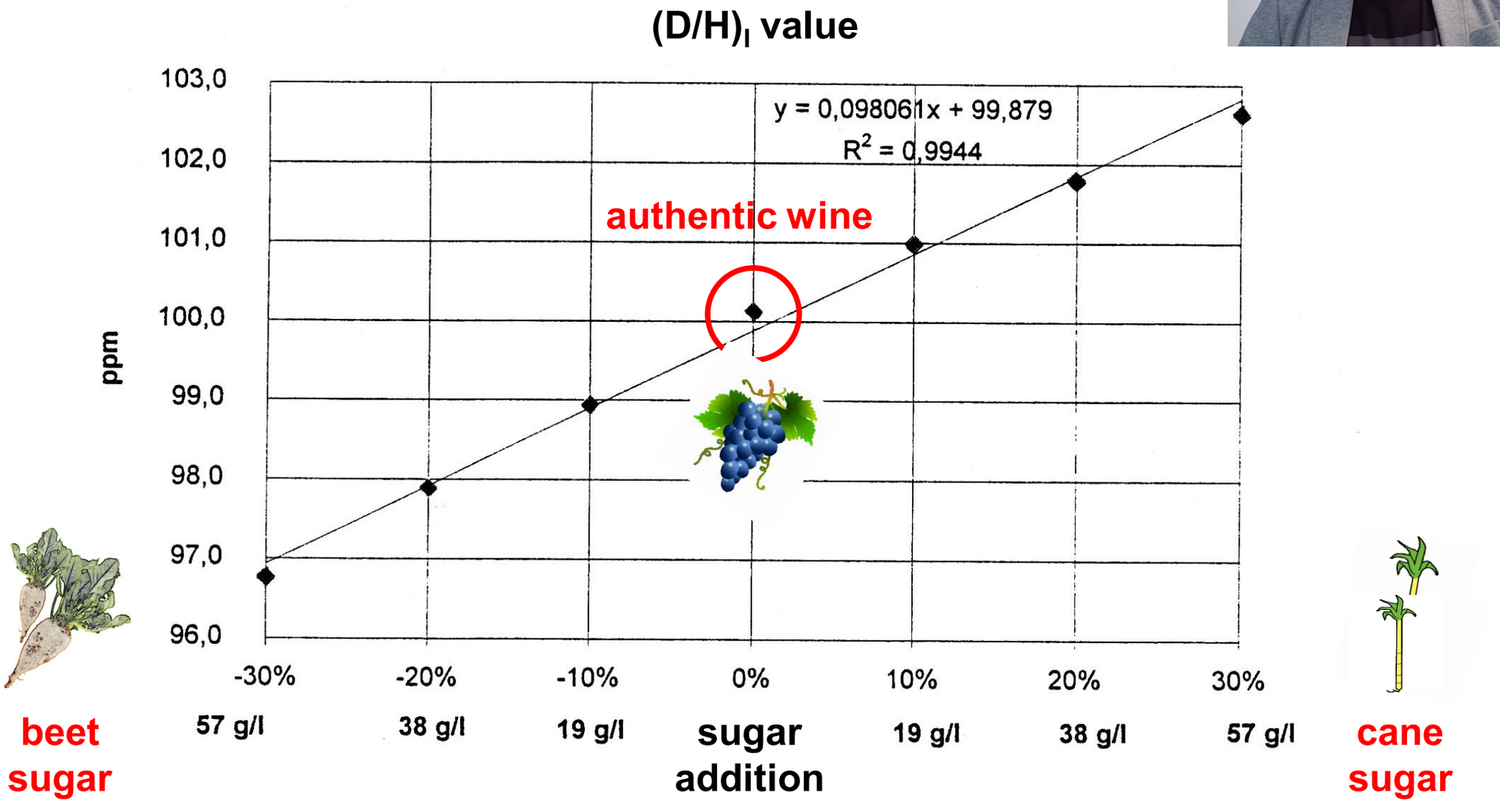
SNIF-NMR measurement

determination of $(D/H)_I$ and $(D/H)_{II}$ values

TMU: Tetramethylurea (internal standard)

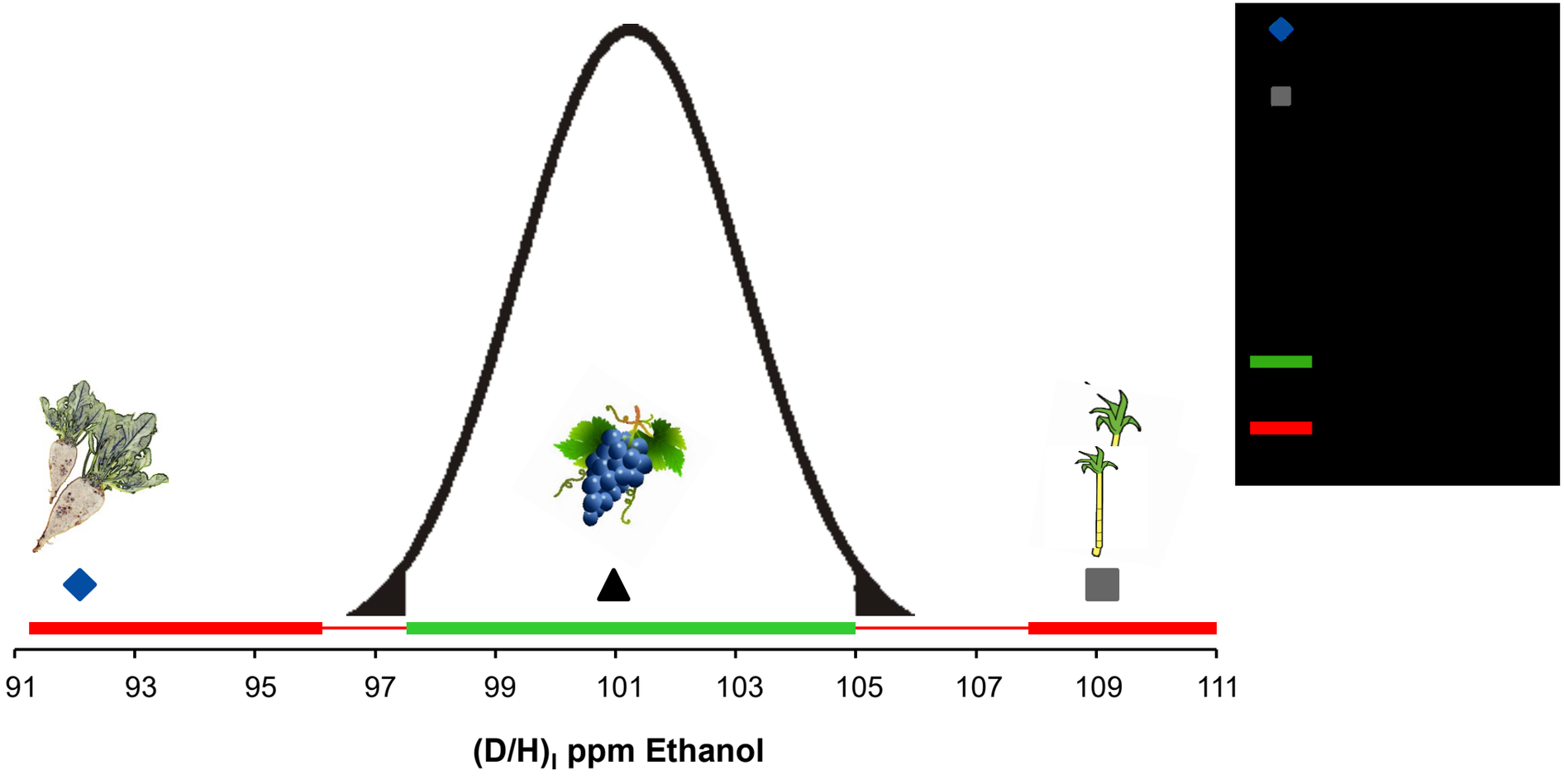
Wine Authentication

- detection of chaptalization/sweetening by **SNIF-NMR spectroscopy**



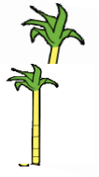
Wine Authentication

- detection of chaptalization/sweetening by **SNIF-NMR spectroscopy**



Stable Isotope Analysis of Wine

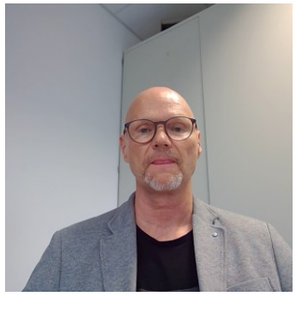
- Official method of OIV to control chaptalization:
  - **D/H isotope ratio in wine ethanol by SNIF-NMR spectroscopy**

    → used to assess addition of beet (C_3) sugar  and cane (C_4) suga 

    → but not mixtures thereof
  - **$^{13}C/^{12}C$ isotope ratio of wine ethanol by IRMS**

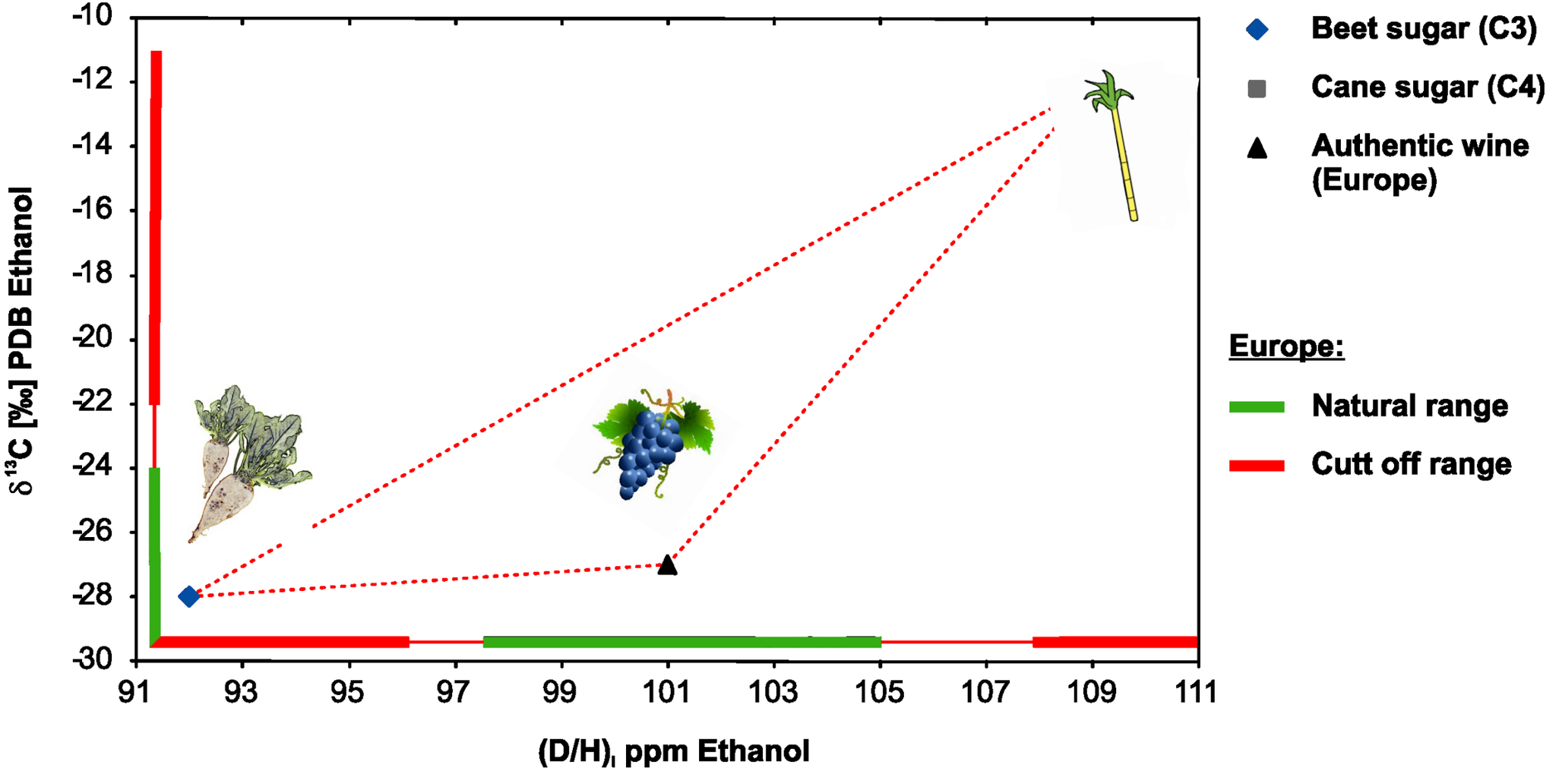
    → used to assess addition of cane (C_4) sugar 
  - Correlation of **D/H** and **$^{13}C/^{12}C$** isotopic data determined by **SNIF-NMR spectroscopy** and **IRMS**, respectively

    → used to assess addition of cane (C_4) sug  nd mixture of sugars 



SNIF-NMR

- Detection of chaptalization/sweetening by SNIF-NMR spectroscopy and ^{13}C IRMS



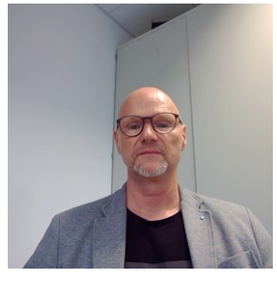
Stable Isotope Analysis of Wine

- **Chaptalization**: Process of adding sugar to unfermented grape must in order to increase the alcohol content after fermentation
- Reg. (EC) No 479/2008:
  - **Zone A** (e.g. most of Germany, UK): **3 % vol.**
  - **Zone B** (e.g. Austria, parts of France): **2% vol.**
  - **Zone C** (e.g. Hungary, parts of Slovakia): **1.5 % vol.**
  - Italy, Greece, Spain, Portugal, Cyprus and parts of France (e.g. Bordeaux): **0 % vol.**

source: wikipedia.org

Jean-Antoine-Claude Chaptal
*1756 – †1832

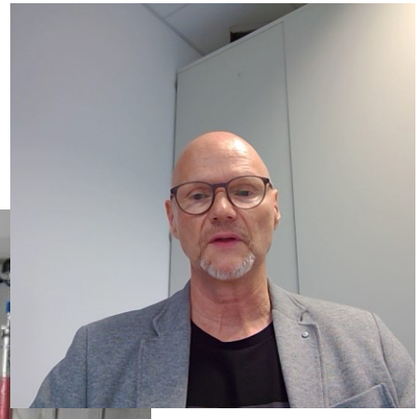
addition of 17 g/L of sugar
=
increase of Alcoholic Grade of 1%Vol

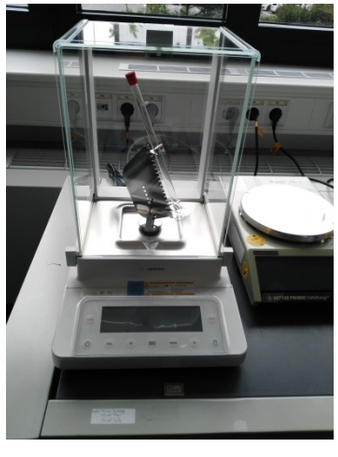


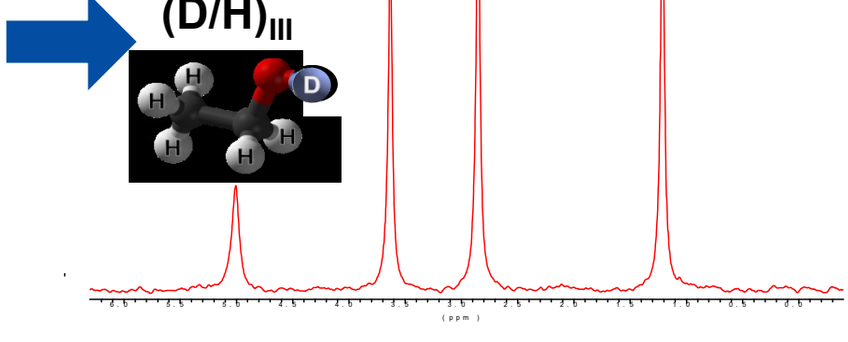
Wine Authentication

COMPENDIUM OF INTERNATIONAL ANALYSIS OF METHODS - OIV
Determination of the deuterium distribution in ethanol by SNIF-NMR

Method OIV-MA-AS311-05 Type II method



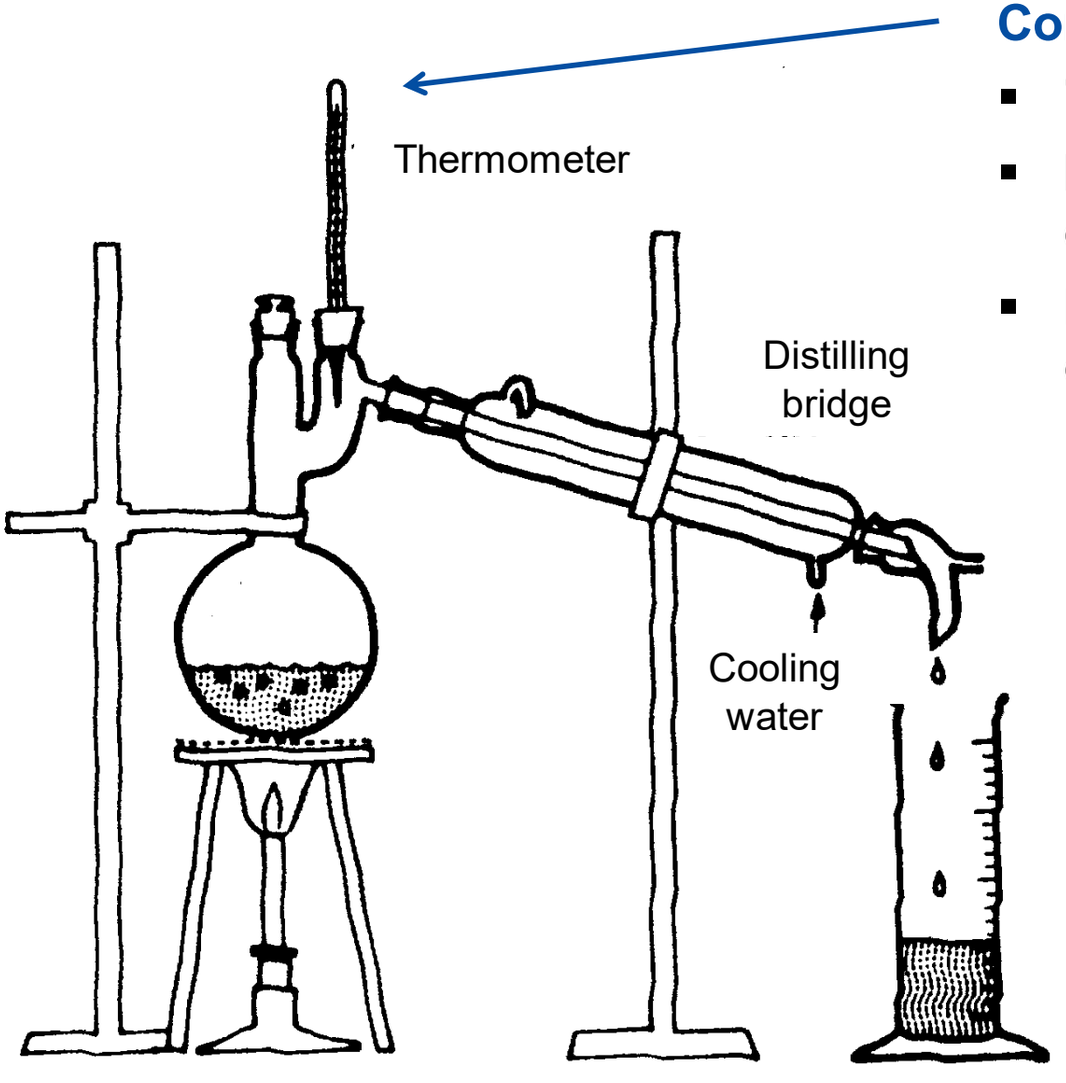




Distillation

COMPENDIUM OF INTERNATIONAL ANALYSIS OF METHODS - OIV
Determination of the deuterium distribution in ethanol by SNIF-NMR

Method OIV-MA-AS311-05 Type II method



250 mL wine

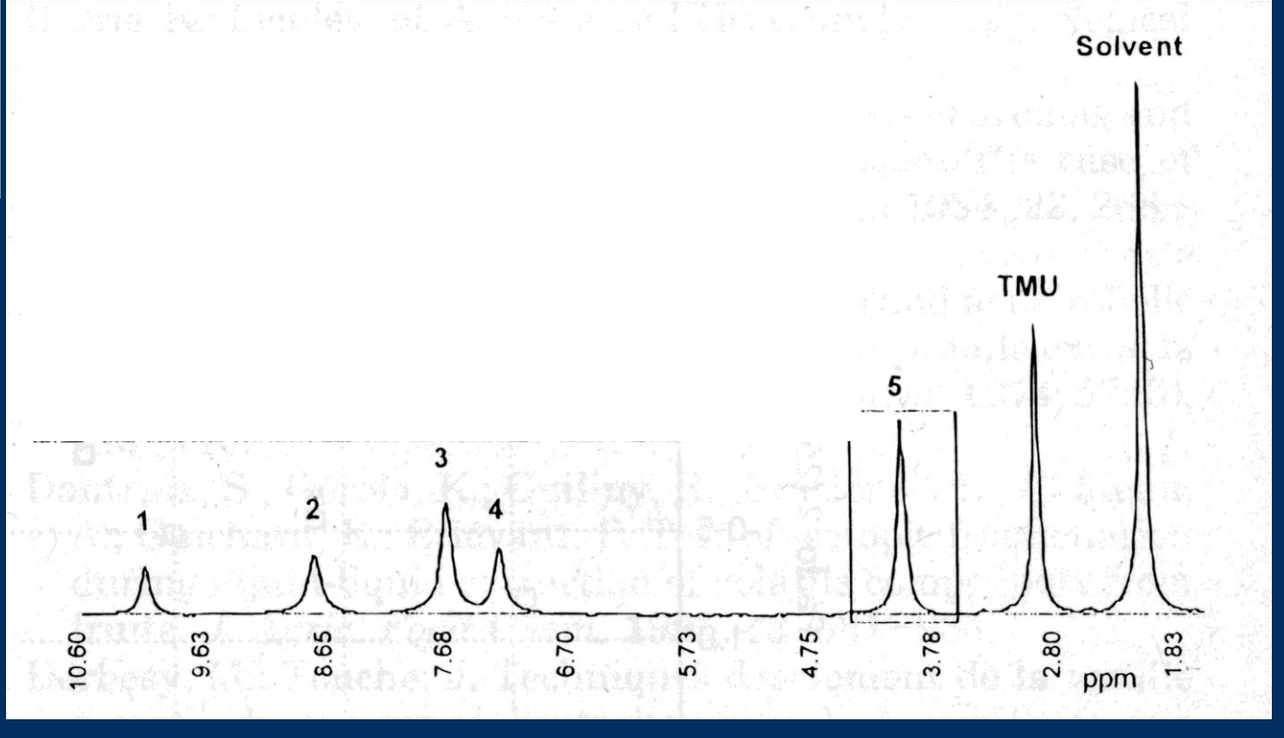
Control temperature!

- **78.0 - 78.2 °C**
- **If > 78.5 °C:** stop destillation, let cool down, start again
- Repeat until temperature does not decrease anymore

Food Identity
(Composition)

Isotopic Analysis

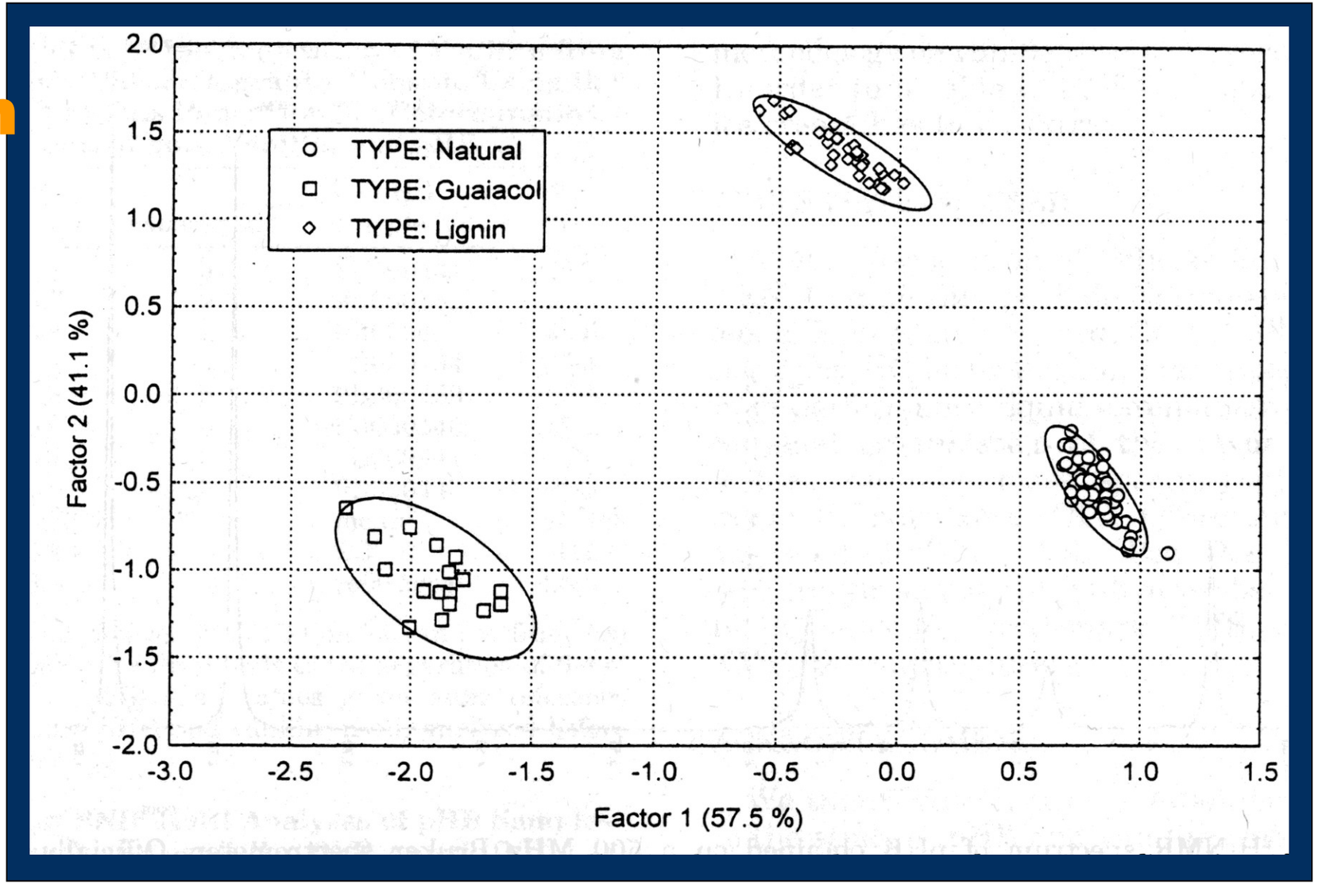
Vanillin



Food Identity
(Composition)

Isotopic Analysis

PCA Vanillin



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Bundesinstitut für Risikobewertung

Thank you for your attention

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