

SNP – W3

Project meeting

Aarhus, 17/11/2022

PhD student: Paraskevi Tsermoula

Supervisor: Bekzod Khakimov

KØBENHAVNS UNIVERSITET



STØTTET AF

Mælkeafgiftsfonden

Foodomics – University of Copen x +


→ ↻ 🏠 🔒 food.ku.dk/english/research_at_food/research_fields/foodomics 🔗 ☆

■ **Department of Food Science** [Department of Food Science](#) > [Research at UCPH FOOD](#) > [Research fields](#) > Foodomics


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The Department of Food Science researches the relationship between food production processes, the composition of food and human health through foodomics


Foodomics is a research discipline that examines the entire set of substances present in our food (foodome). The discipline uses advanced analytical platforms to investigate the composition of the food and thus, its nutritional properties and impact on health. The new techniques also provide a detailed picture of food quality and can be used to detect food fraud and to find solutions for other challenges in food production. Research results from foodomics have a direct impact on consumers, the food industry and society.





Contact

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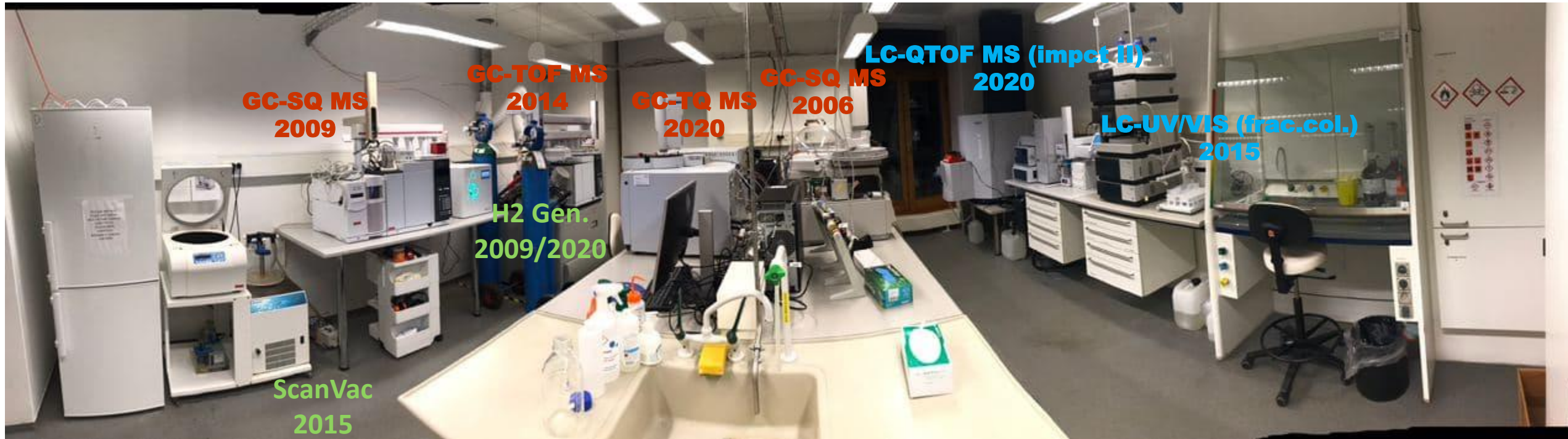
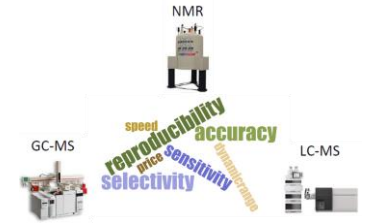
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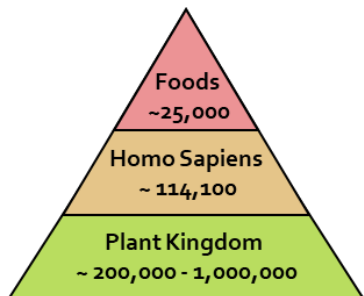
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KU.FOODOMICS CHROMATOGRAPHY LABORATORY (R443)



uncover "dark matter"



CURRENT FOCUS

Plants
Plant Foods

Beverages
Dairy Products
Fermented Food

Bioactives
Vitamins
Essential AAs

Proteins
Dietary Fibers
Microbial origin

Contaminants
Adulterants
Antinutrients

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Research Interests

Analytical Chemistry – Foodomics - Multivariate Data Analysis

I am interested in extending the boundaries of analytical chemistry methods to screen small molecular metabolites in biological systems prior to understand their responses to external factors.

Three major analytical platforms I work:

- 1) Nuclear Magnetic Resonance Spectroscopy (NMR)
- 2) Gas Chromatography-Mass Spectrometry (GC-MS)
- 3) Liquid Chromatography-Mass Spectrometry (LC-MS)

Current Research Projects

- 1) Introduction of statistical causality modelling and deep learning to solve the cage of covariance problem in Foodomics/Metabolomics, Source of funding: *UCPH*
- 2) Aging of Biological Traces: A Forensic Application TraceAge (TraceAge), Source of funding: *Innovation Fund Denmark*
- 3) Low molecular weight compounds in milk and dairy streams - a potential new source for value added products (MilkStreamValue), Source of funding: *Danish Dairy Research*

Foundation

Teaching

Responsible

Foodomics and Plant Foods, Full Degree Master Course, 7.5 ECTS

Teacher

Thematic Course in Food Science and Technology, Full Degree Master Course, 7.5

ECTS

Teacher

Quantitative Bio-spectroscopy, Full Degree Master Course, 7.5 ECTS

Teacher

Advanced Carbohydrate Technologies. , Full Degree Master Course, 7.5 ECTS

Responsibilities

Responsible

Analytical Chemistry Platforms - three high-throughput GC-MS and two LC-MS

(UV/Vis)

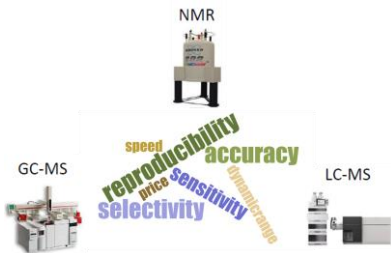
systems in Foodomics Laboratory

Co-responsible

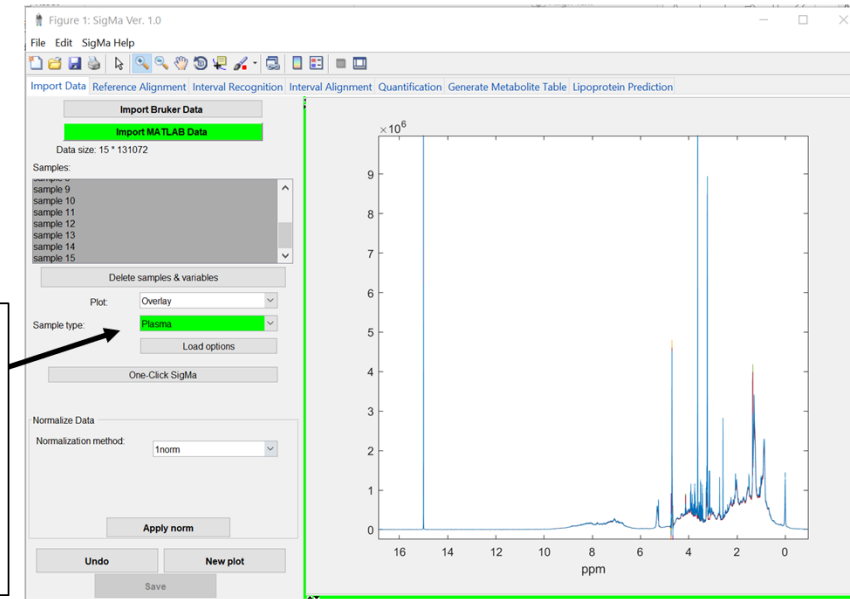
Three Nuclear Magnetic Resonance (NMR) Spectrometers (600, 500, and 400 MHz) in

CPSC

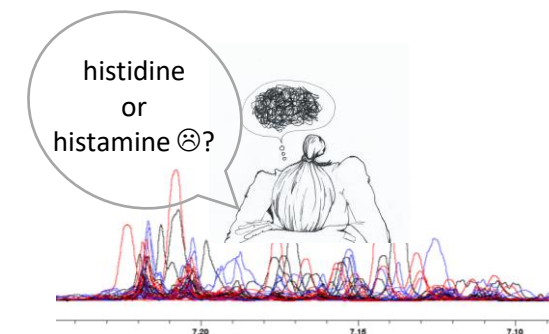
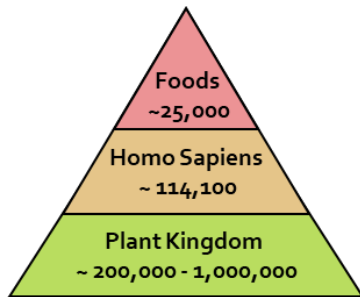
1ST. ASSOCIATE PROFESSOR IN FOODOMICS



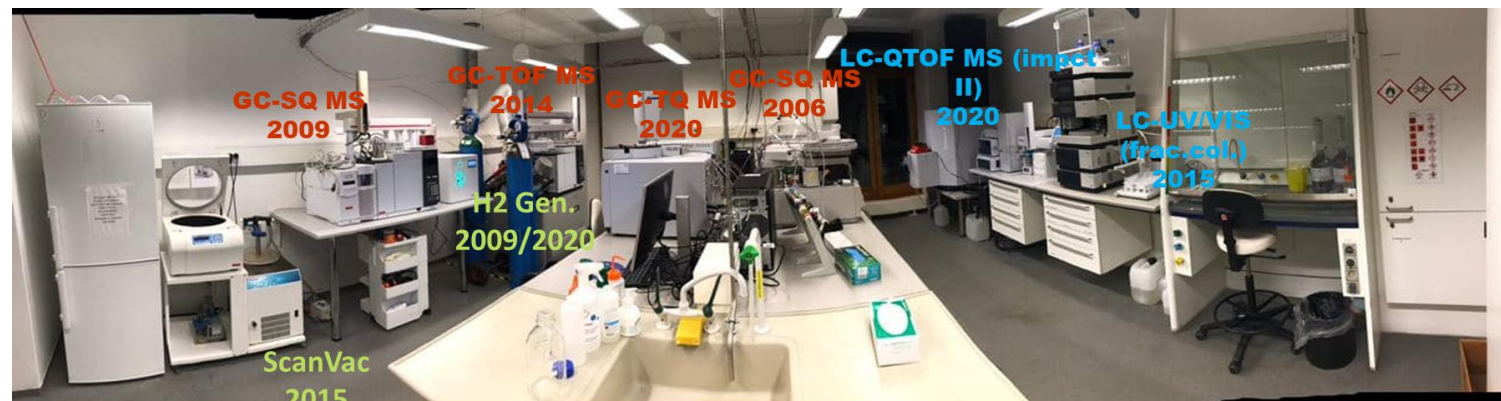
- a mouse click away metabolite table-



uncover "dark matter"



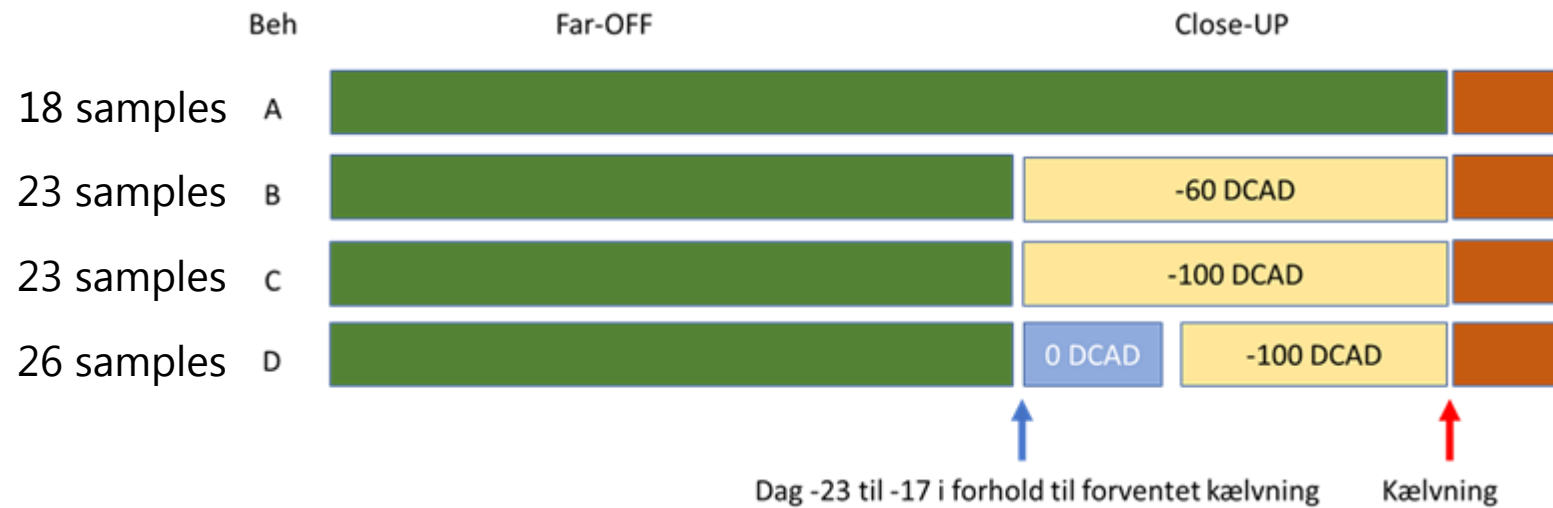
Khakimov et al., *Analytica Chimica Acta* 1108 (2020) 142-151



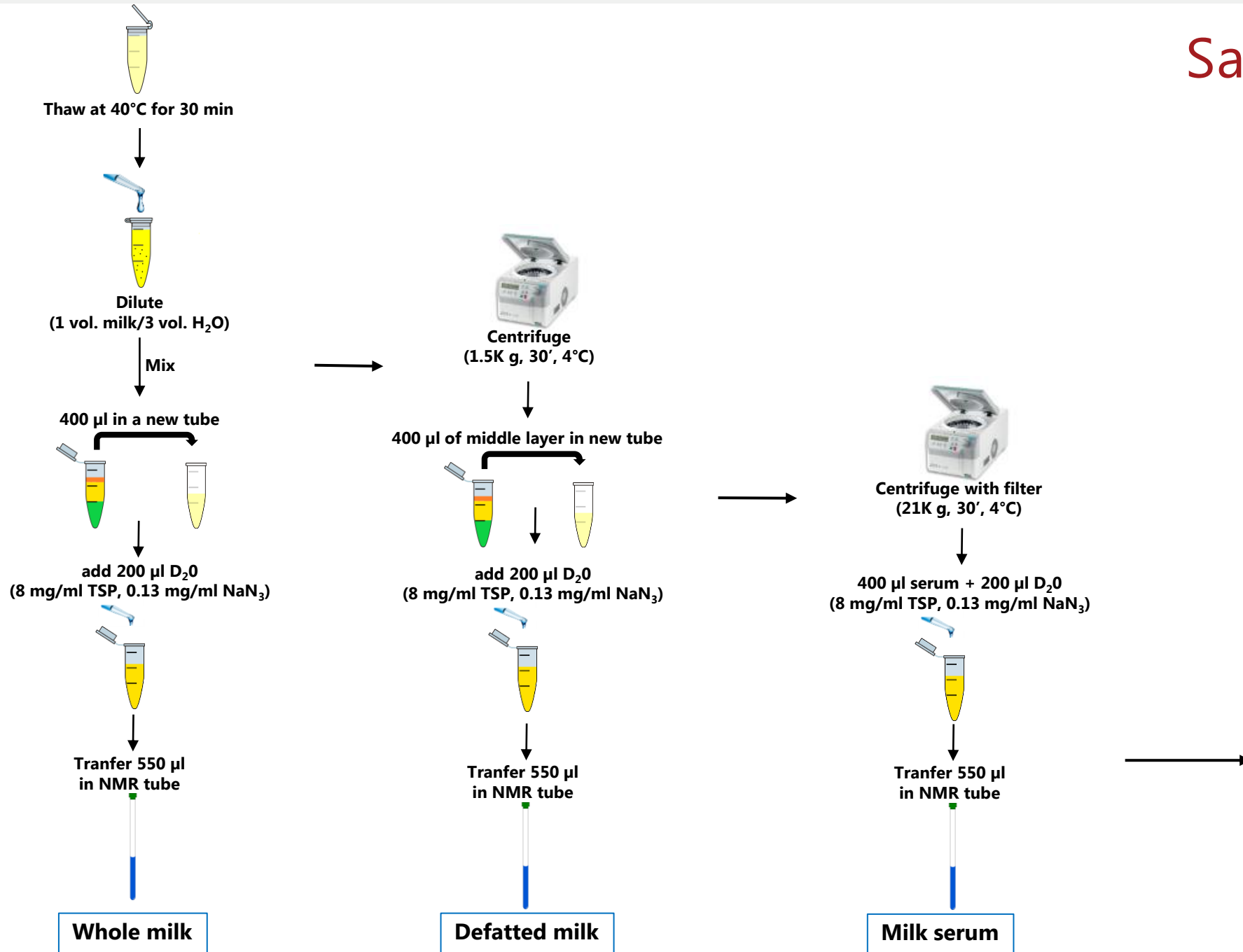
Aim

- To characterize the molecular composition of bovine colostrum.
- To identify markers that reflect the physiological status of the cows during the period around calving.

Colostrum milk samples



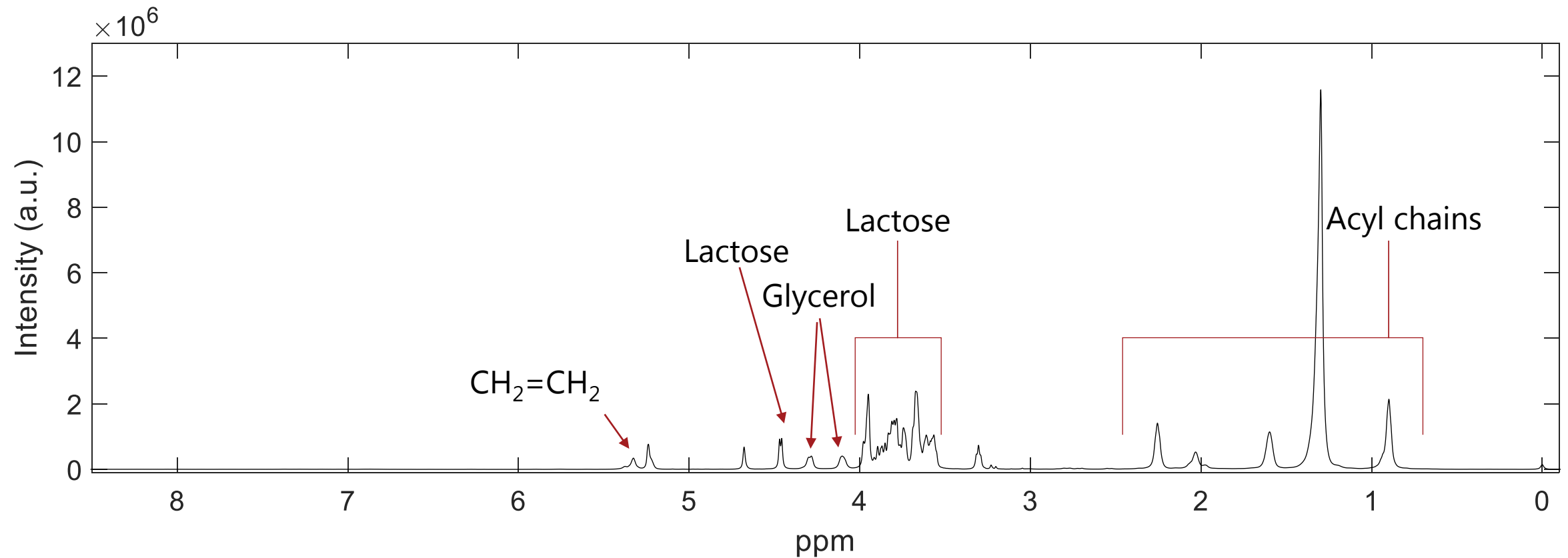
Sample preparation



Measure

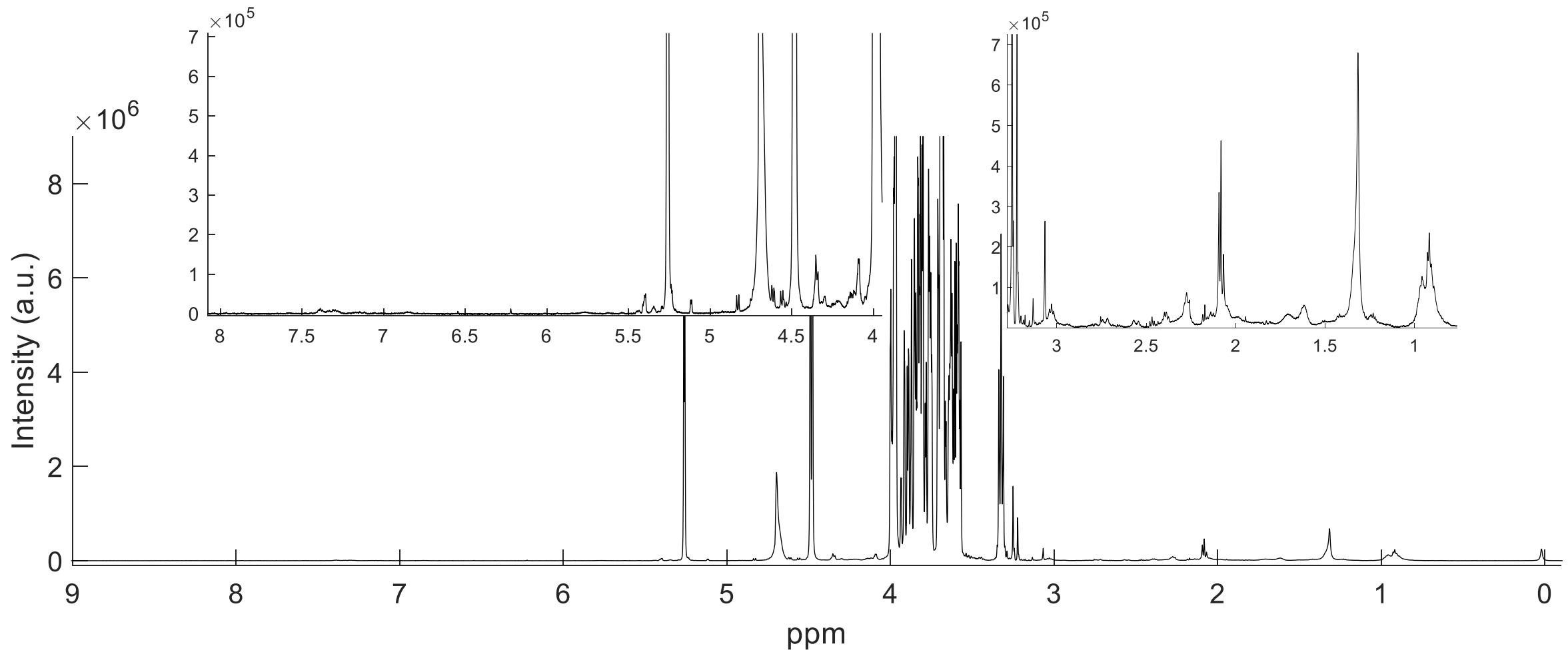
Whole milk ^1H NMR spectrum

✓ Milk fingerprint



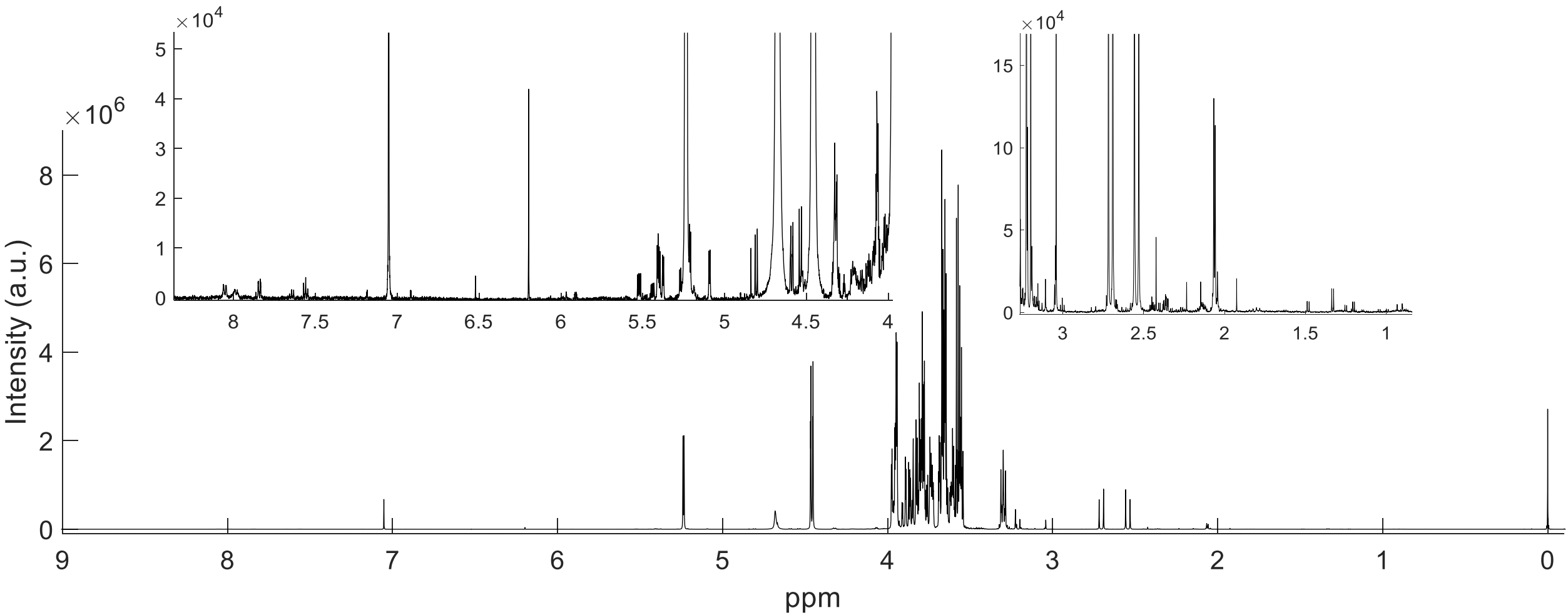
Defatted milk ^1H NMR spectrum

✓ High-throughput and more sensitive

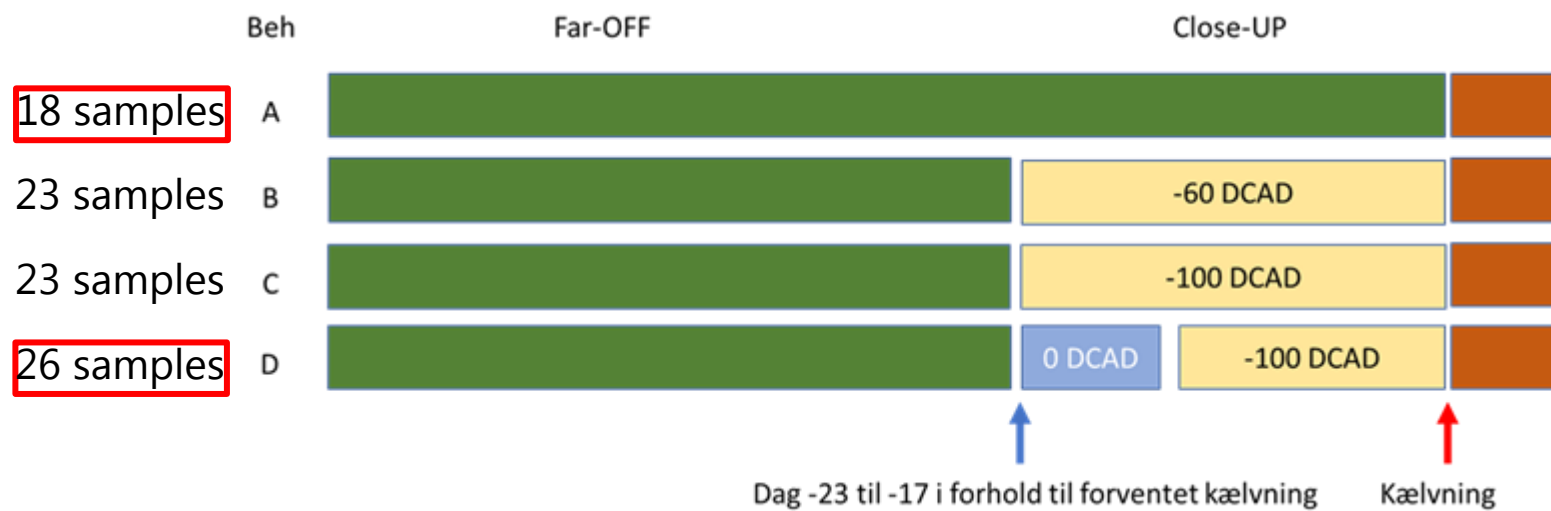


Milk serum ^1H NMR spectrum

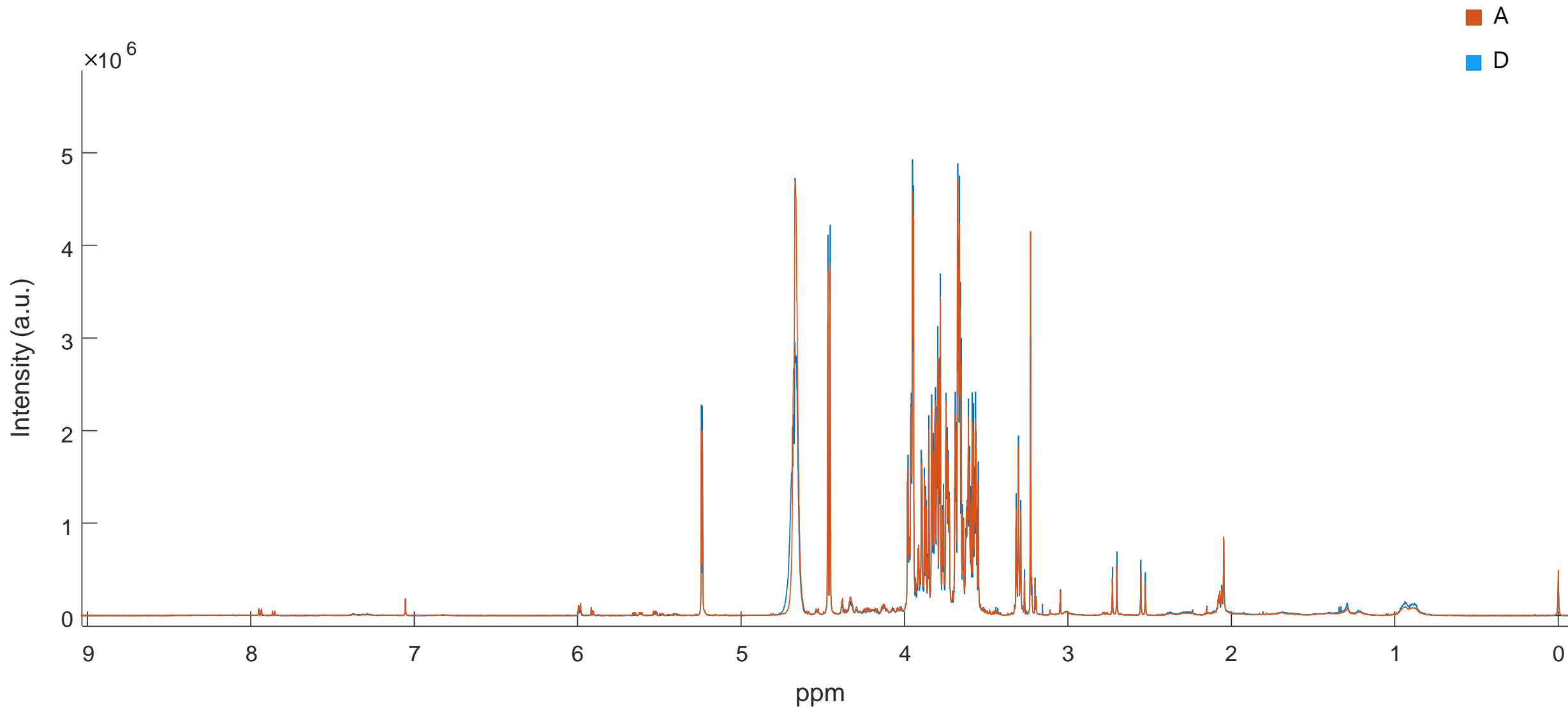
✓ More time consuming and the most sensitive



Colostrum milk samples



^1H NMR spectra of defatted colostum from A and D groups



¹H NMR spectra of defatted colostum from A and D groups

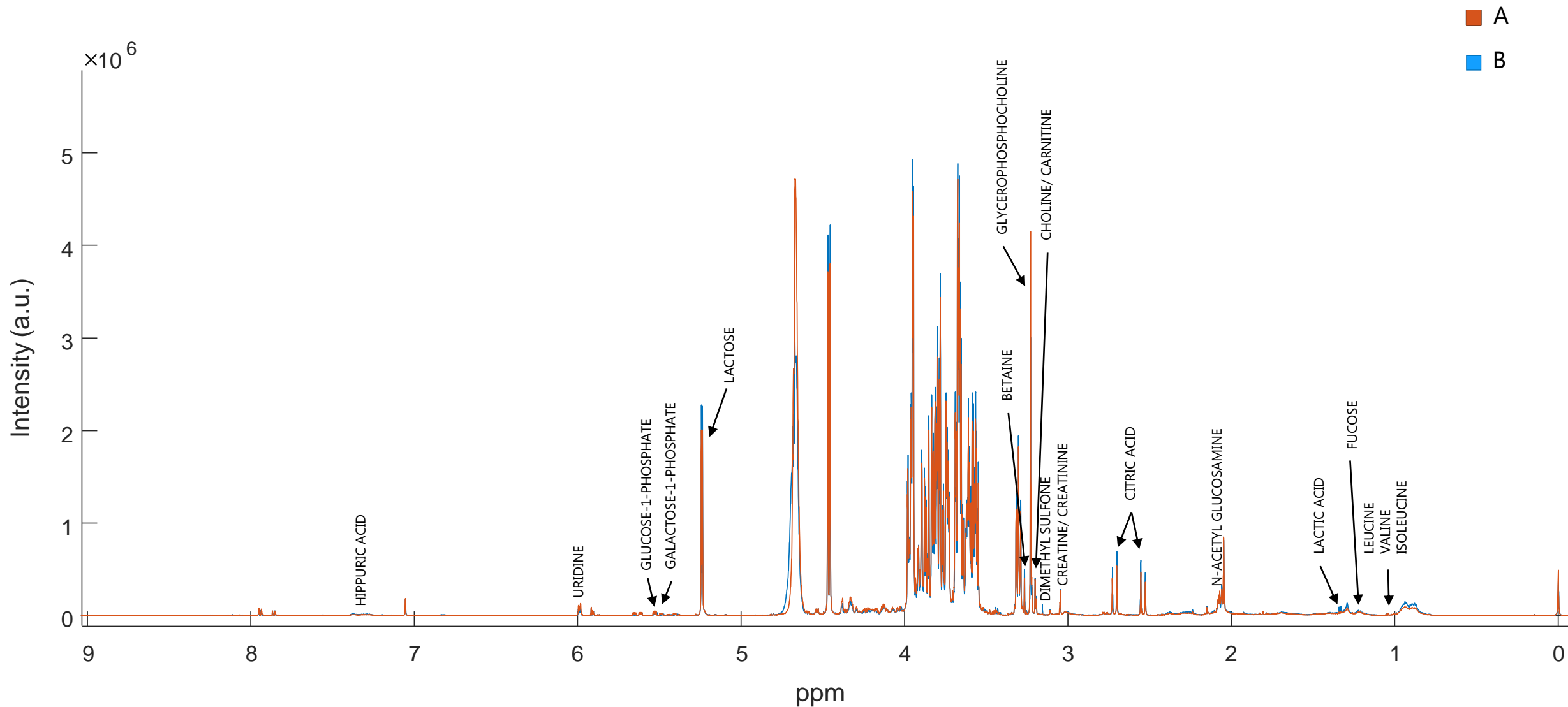
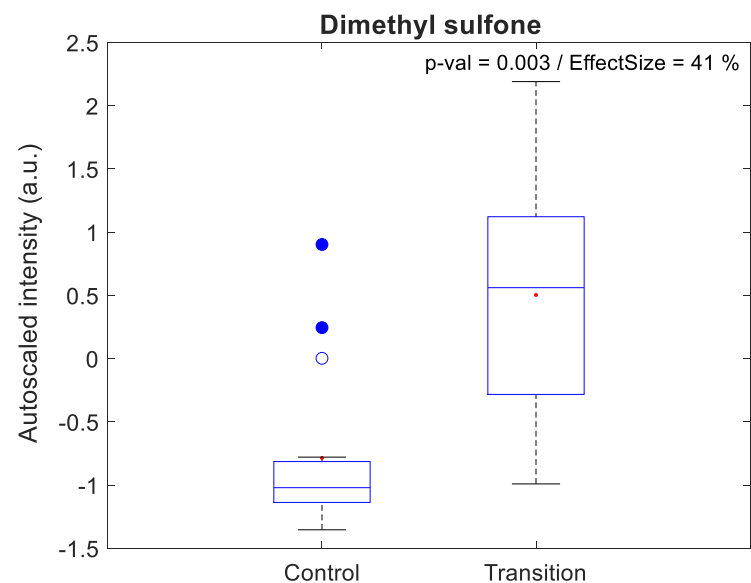
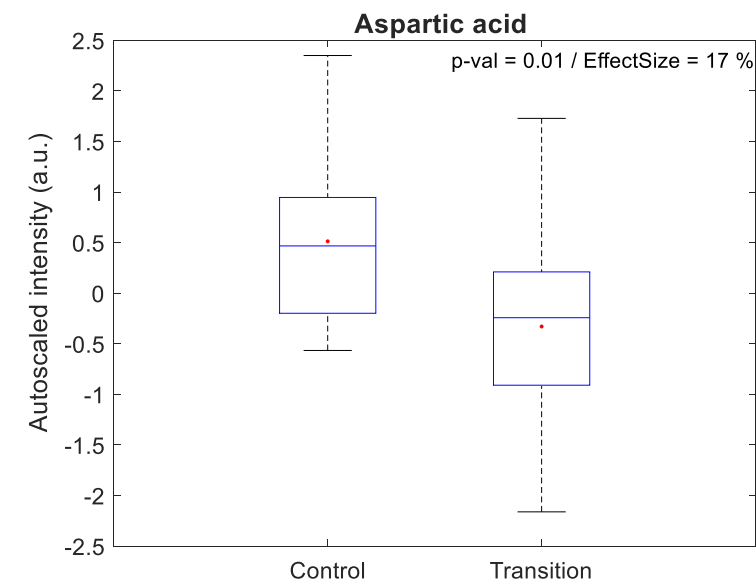
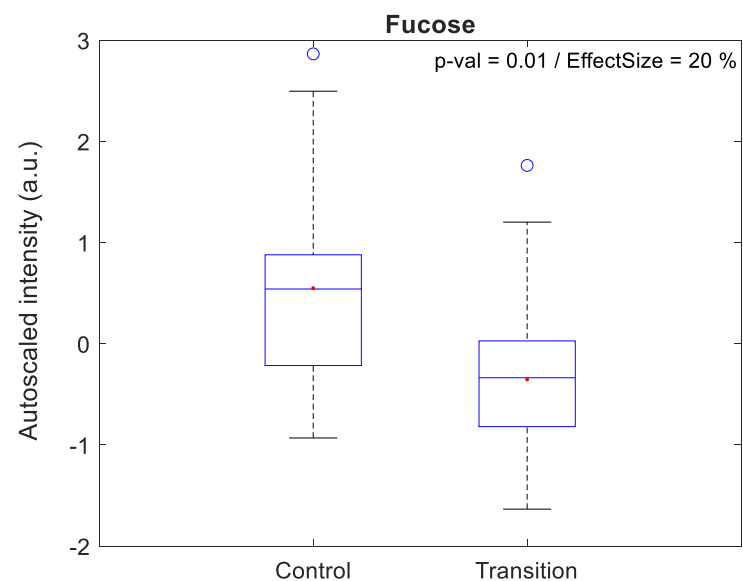
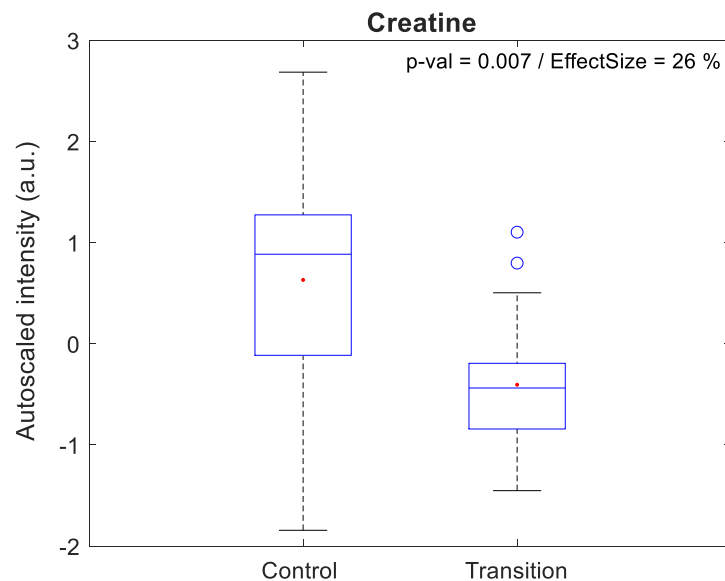


Table of identified metabolites

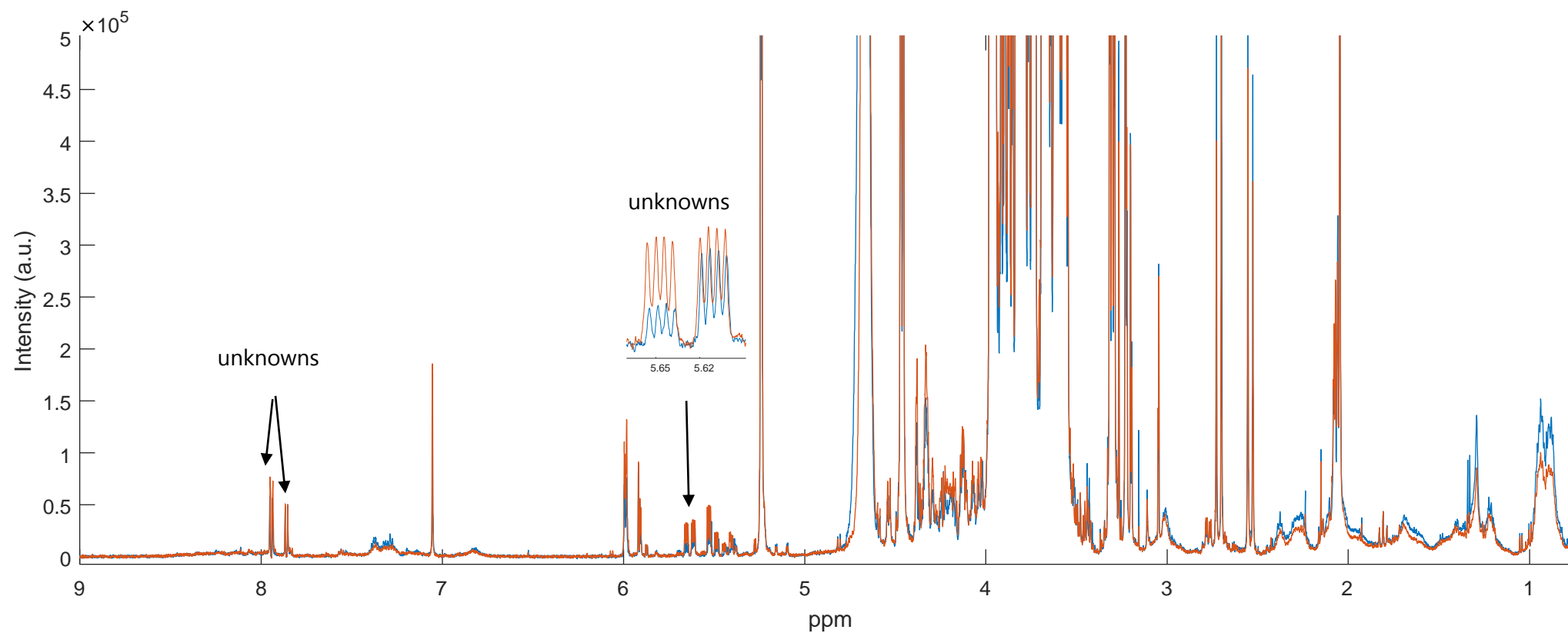
Interval name	Chemical shift (ppm)	Multiplicity	Type of protons
1 pantothenic acid	0.95	s	CH ₃
2 leucine	0.97	t	CH ₃
3 valine	0.99	s	CH ₃
4 isoleucine	1.02	d	CH ₃
5 fucose	1.26	d	CH ₃
6 lactic acid	1.34	d	CH ₃
7 alanine	1.49	d	CH ₃
8 acetic acid	1.93	s	CH ₃
9 n-acetyl glucosamine	2.06	s	CH ₂
10 acetylcholine	2.15	s	CH ₃
11 acetoacetic acid	2.24	s	CH ₃
12 malic acid	2.36	d	CH ₃
13 carnitine	2.42	s	CH ₂
14 dimethylamine	2.50	s	CH ₂
15 citrate	2.55	d	2 × -CH ₂
16 methylamine	2.60	s	CH ₂
17 aspartic acid	2.68	dd	CH ₃
...			
39 cytidine	6.07	d	-CH
40 orotic acid	6.20	s	-CH
41 fumaric acid	6.53	s	-CH
42 tyrosine	6.91	d	2 × -CH
43 uracil	7.06	d	N-CH
44 tryptophan	7.54	d	N-CH
45 hippurate	7.56	m	-CH, 2 × CH ₂
46 uridine	7.64	t	-CH
47 formic acid	7.86	s	-CH
18 unknowns			
9 BINS			

Discriminating metabolites



^1H NMR spectra of defatted colostum

■ A
■ B



Standard addition experiment (66 compounds) – In progress

2-oxoglutaric acid	Ethanolamine	L-leucine
Acetic acid	Formic acid	L-tryptophan
Acetoacetic acid	Fumarate	L-tyrosine
Acetone	Galactose 1-phosphate	L-valine
Acetylcholine	Glucose-1-phosphate	Malate
Adenine	Glutamine	Malonic acid
Betaine	Hippuric acid	Methanol
Butyric acid	Isobutyric acid	Methionine
Capric acid	Isopropanol	Methylamine
Caprylic acid	Isovaleric acid	N-acetylglucosamine
Choline	L-acetylcarnitine	Niacinamide
Cis-aconitic acid	Lactose	O-phosphocholine
Citric acid	L-alanine	Oxaloacetic acid
Citrulline	L-arginine	Pantothenic acid
Creatine	L-asparagine	Phenylalanine
Creatine-1-phosphate	L-aspartic acid	Propionic acid
Creatinine	L-carnitine	Pyruvic acid
Cytidine	L-fucose	Succinic acid
D-galactose	L-glutamic acid	Trimethylamine
D-glucose	L-histidine	Uracil
Dimethyl sulfone	L-isoleucine	Urea
Dimethylamine	L-lactate	Uridine

In progress

- Finalise analysis of whole, defatted and serum colostrum
- Possible identification unknown peaks
- Identify possible discriminating metabolites among A, B, C and D colostrum samples

Future plans

- To analyze cows' urine metabolome with the objective to identify markers that reflect the physiological status of the cows around the period calving period.

SigMa: Signature Mapping



➤ A new approach for processing complex NMR spectra of mixtures

