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Atypical Spectra Screening: Applications for Monitoring Infrared Instruments and Model Predictions

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Data scientist, Innovation and Business Development Qlip

ICAR 2021

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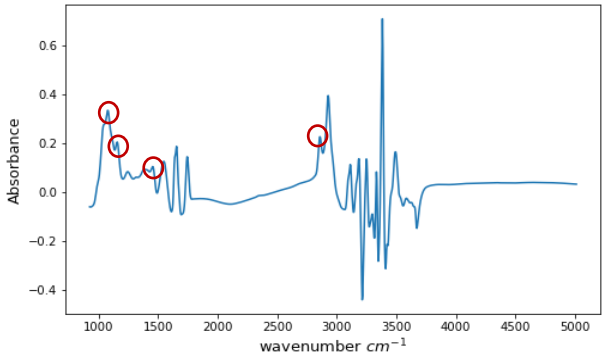
Background

Milk sample

FT-IR spectrometer

FT-IR milk spectrum



- **F**ourier-**T**ransform mid **I**nfra**R**ed spectrometry (FT-IR) of liquid milk
- Composition milk profile predicted (i.e., calculated) from IR spectrum

Mathematical prediction model

4.3% fat
3.4% protein
4.5% lactose

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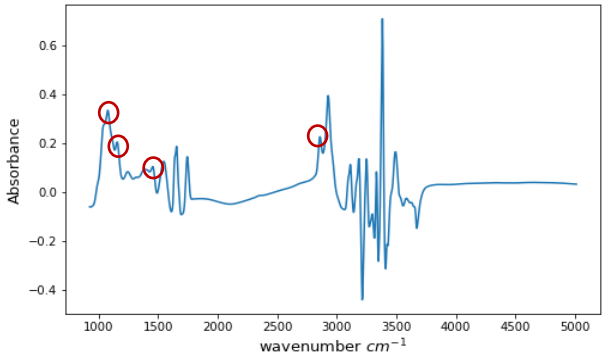
Milk sample

IR spectrometer

FT-IR milk spectrum



- Quality of predictions dependent on:
  - Quality of the model (e.g., robustness)
  - Quality of the spectra (noise and artifacts)

Mathematical prediction model

4.3% fat
3.4% protein
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Background

- Each spectrum results from **measurement process** performed under…
    - specific conditions
    - using a specific IR instrument

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Background

- Each spectrum results from **measurement process** performed under…
  - specific conditions
  - using a specific IR instrument

- Changes in measurement process (e.g., instabilities in the IR instrument) can lead to changes in the spectra

- **Problematic**:
  - …if this happens in spectral regions containing chemical information used by prediction models
  - …because the instrument is not working properly

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Background

Slope / intercept correction

- ✓ Fat
- ✓ Protein
- ✓ Lactose

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Background

- Limited use-case for slope / bias corrections

Slope / intercept correction

	✓ Fat	✗ Pasture intake
	✓ Protein	✗ Methane emissions
	✓ Lactose	✗ NEFA, BHB_{Blood}
Present in control milk?	✓	✗

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Background

- Limited use-case for slope / bias corrections

- **We need a general approach for monitoring the quality of our data (spectra, predictions)**

Slope / intercept correction

	Fat	Pasture intake
	Protein	Methane emissions
	Lactose	NEFA, BHB
Present in control milk?	✓	✗

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Background

- Limited use-case for slope / bias corrections

- **We need a general approach for monitoring the quality of our data (spectra, predictions)**

- Monitor spectra for systematic deviations due changes in the measurement process (i.e., instrument instabilities).

    - Use mathematical models originally developed to screen for non-specific adulteration in milk samples

Slope / intercept correction

	✓ Fat	✗ Pasture intake
	✓ Protein	✗ Methane emissions
	✓ Lactose	✗ NEFA, BHB
Present in control milk?	✓	✗

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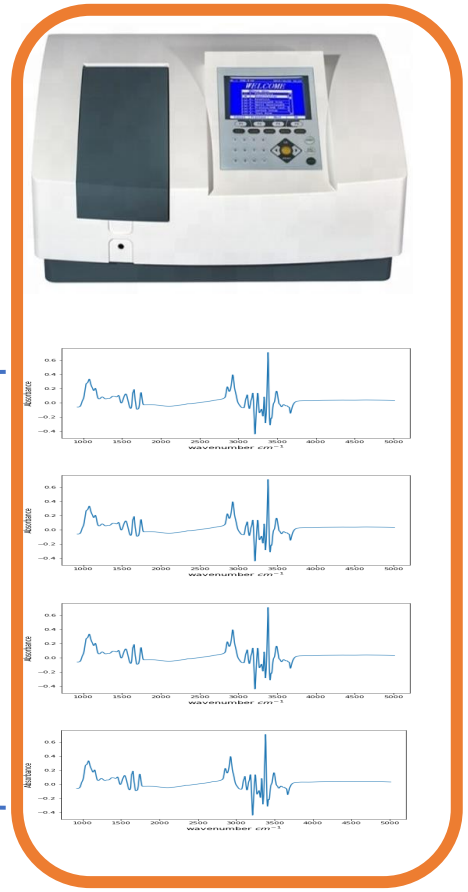
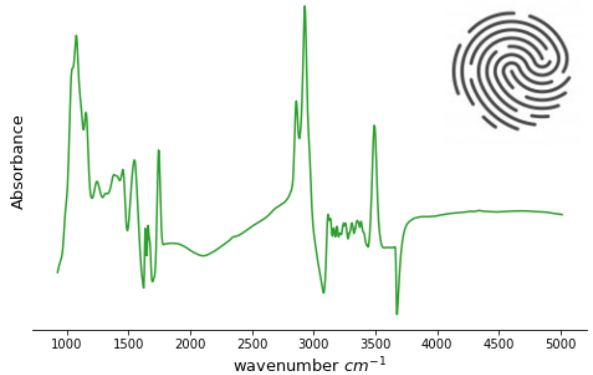
Methods & Results

Milk spectra with normal variation



Instrument-specific milk fingerprint



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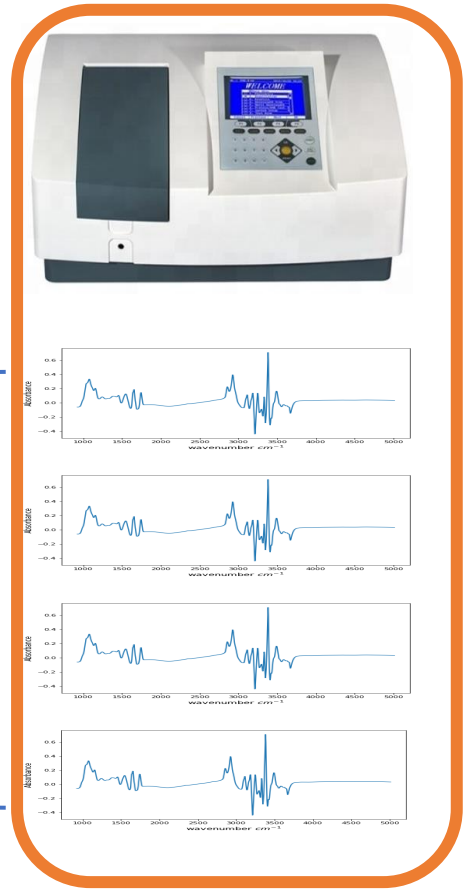
Methods & Results

Milk spectra with normal variation



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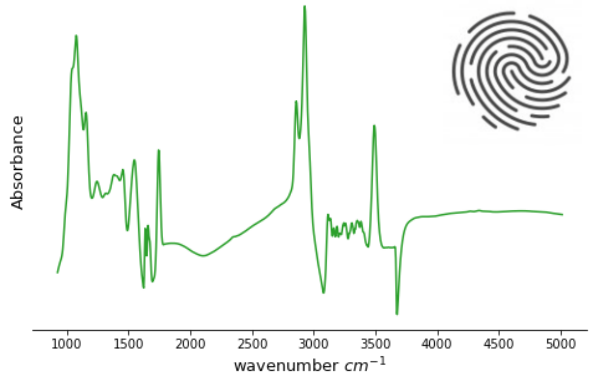
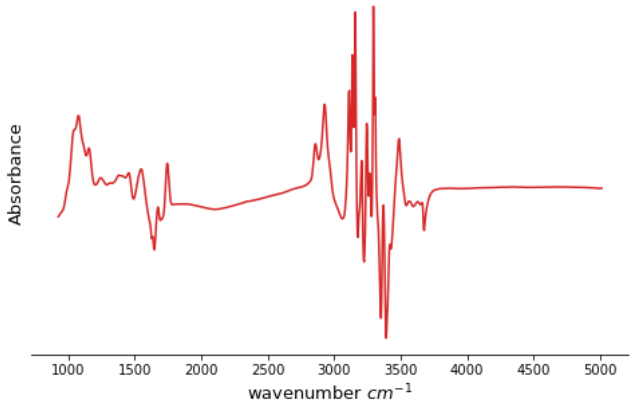


vs.

New spectrum from same instrument



Compute anomaly scores for each spectrum from the same instrument

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Methods & Results

- Compute anomaly scores for each spectrum from the same instrument
- **Look for patterns over time**

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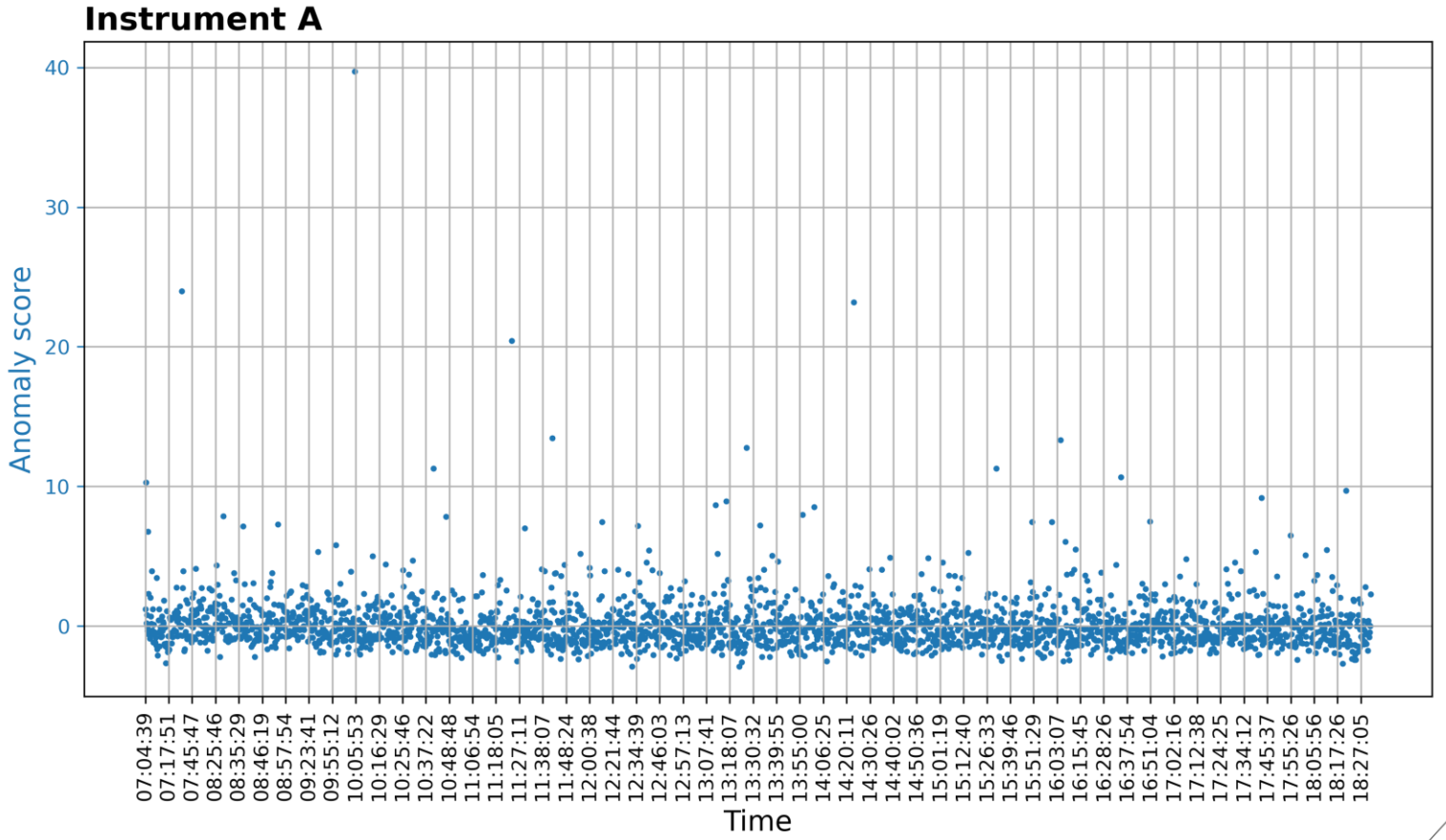

No pattern; mostly random noise with zero mean

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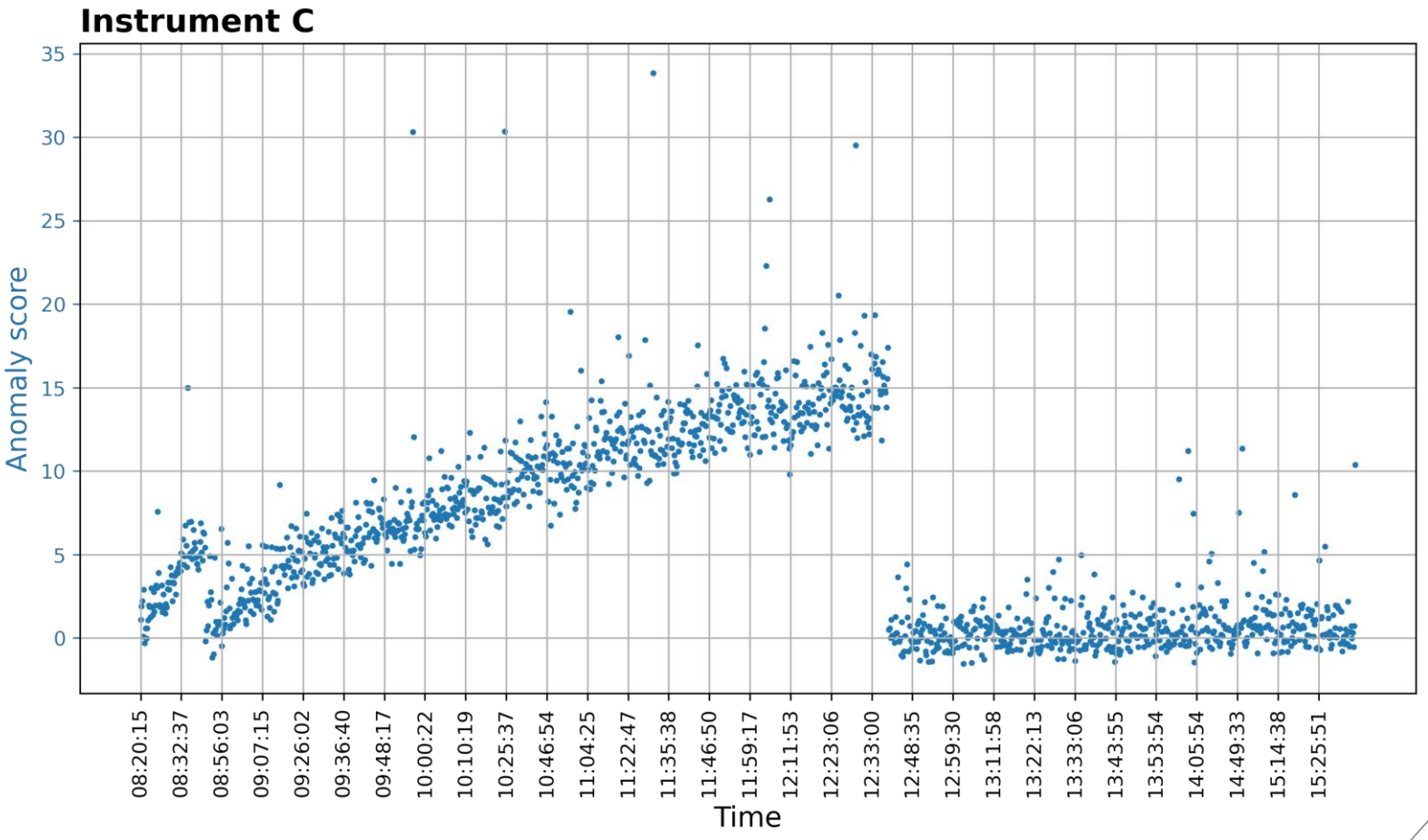

Gradual increase of anomaly scores

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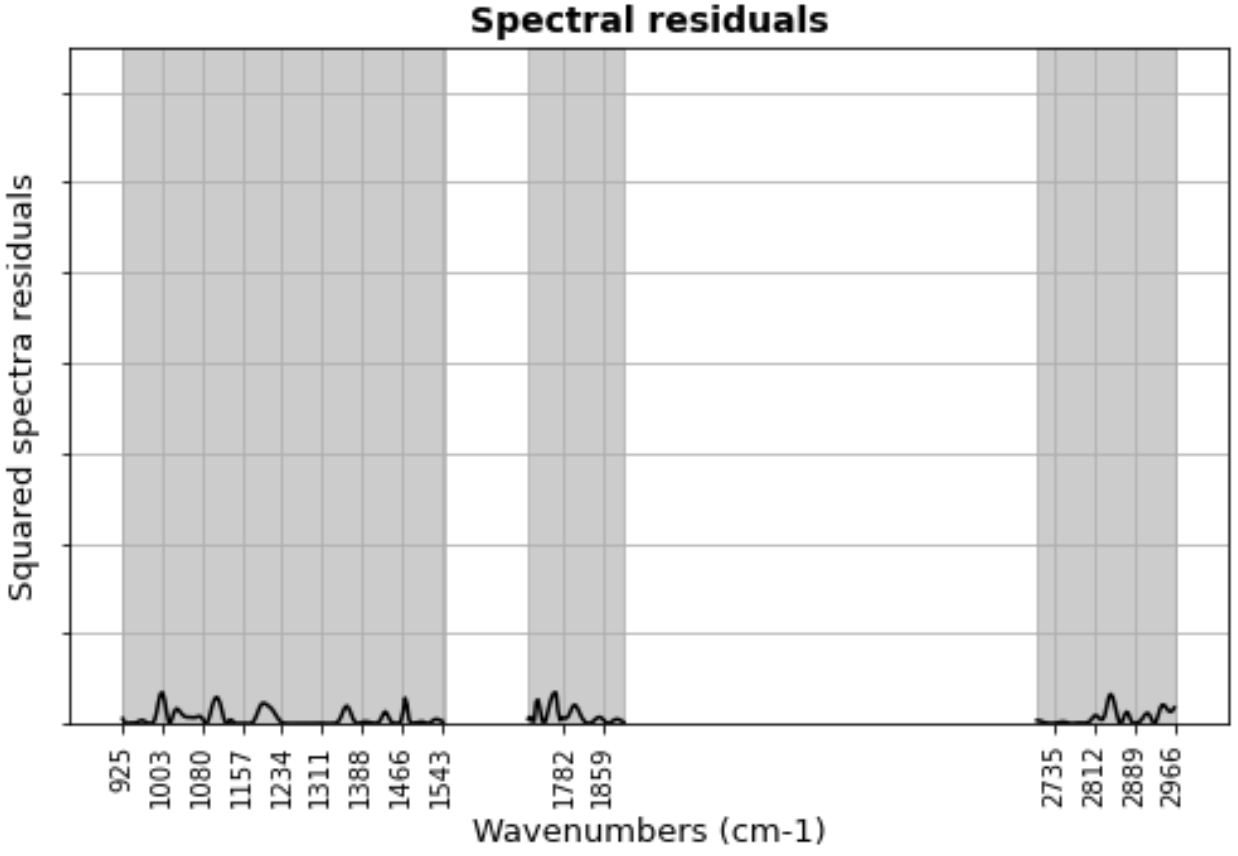

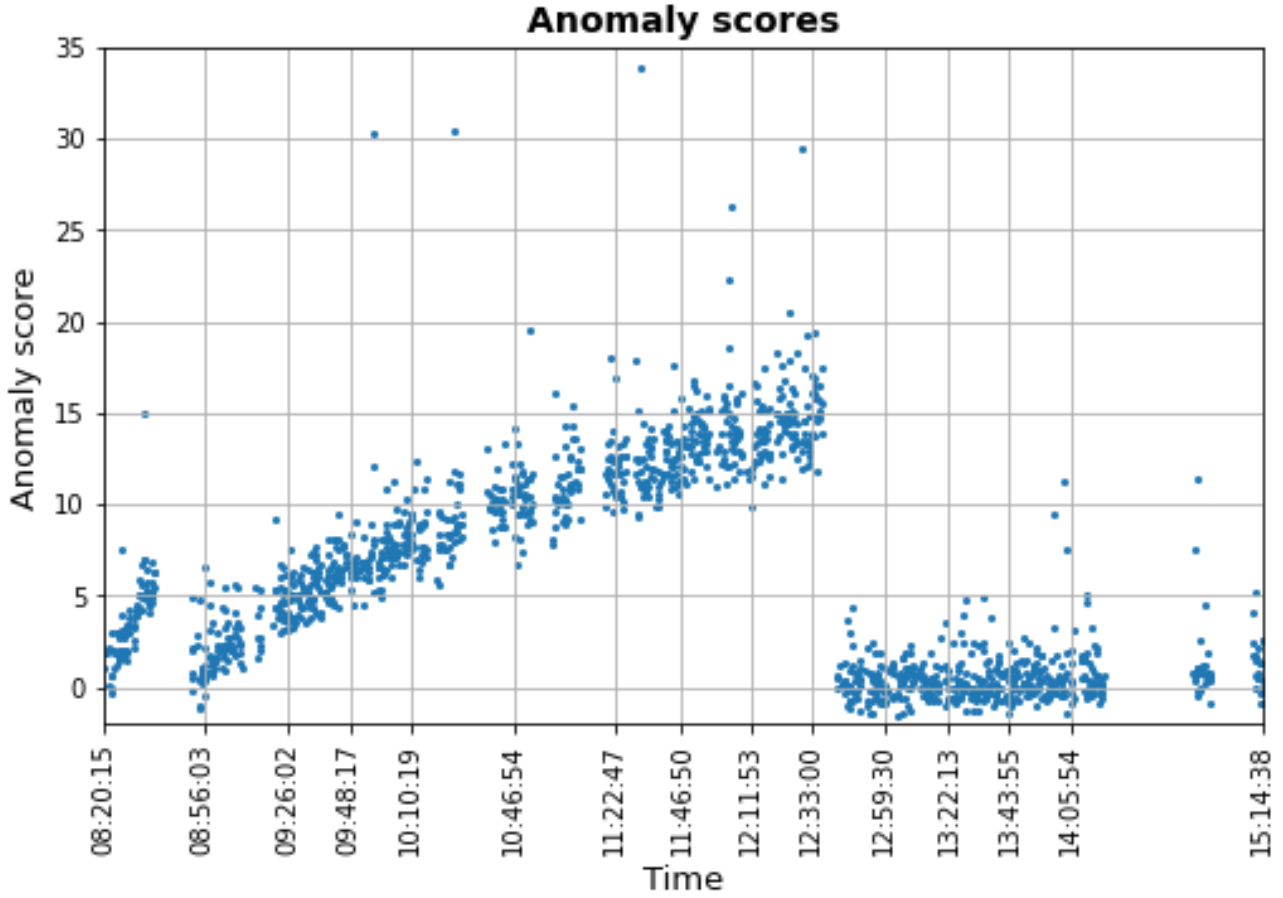

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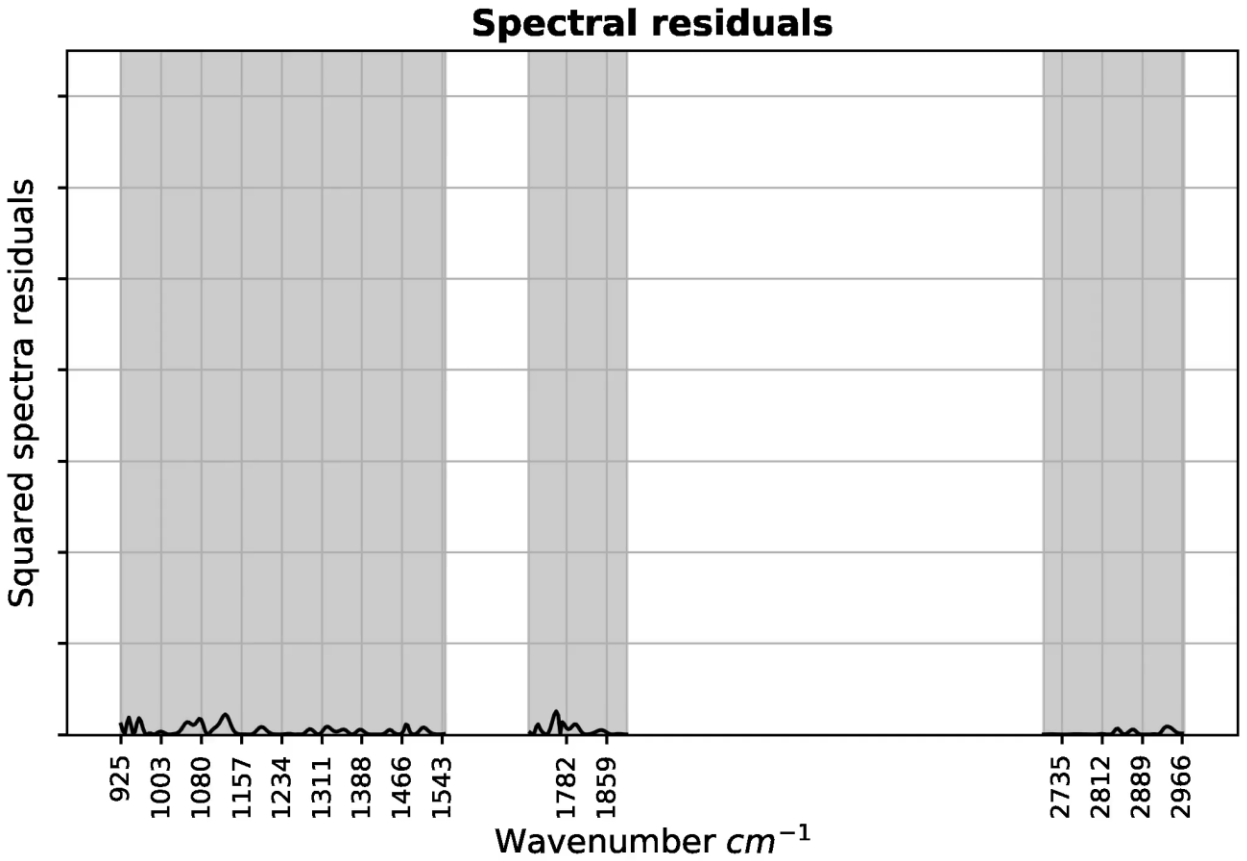

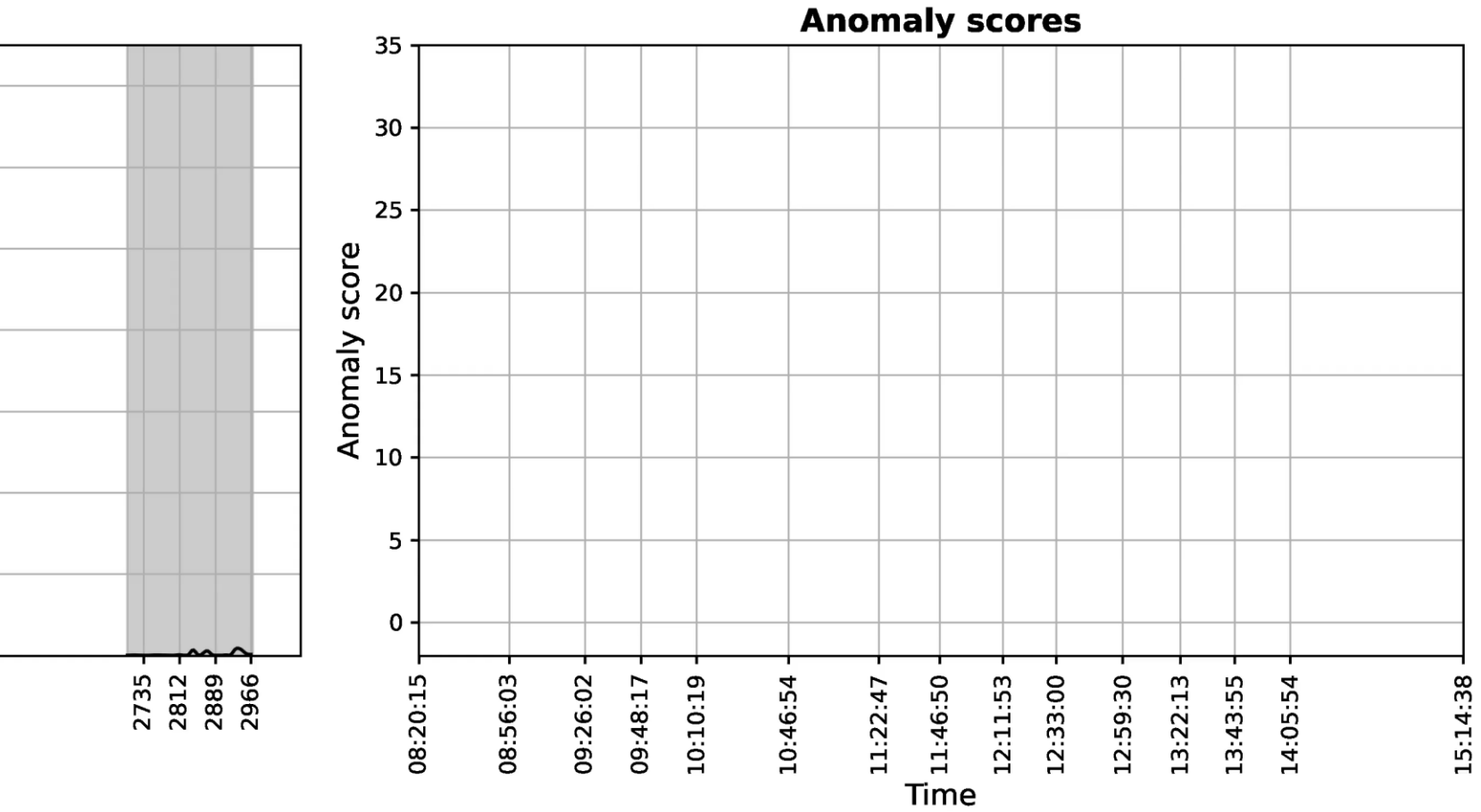

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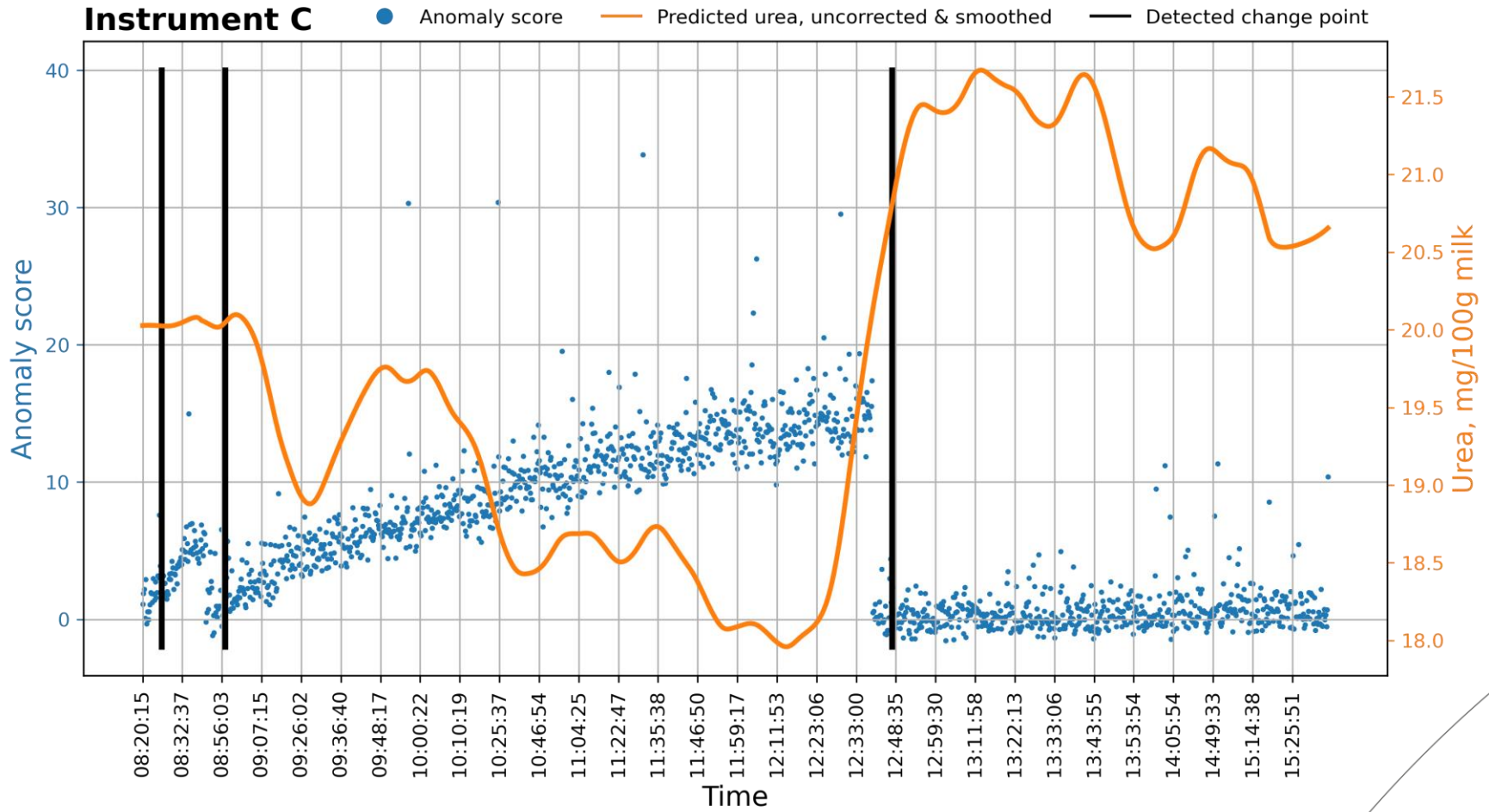

Change in anomaly scores coincides with bias in urea predictions

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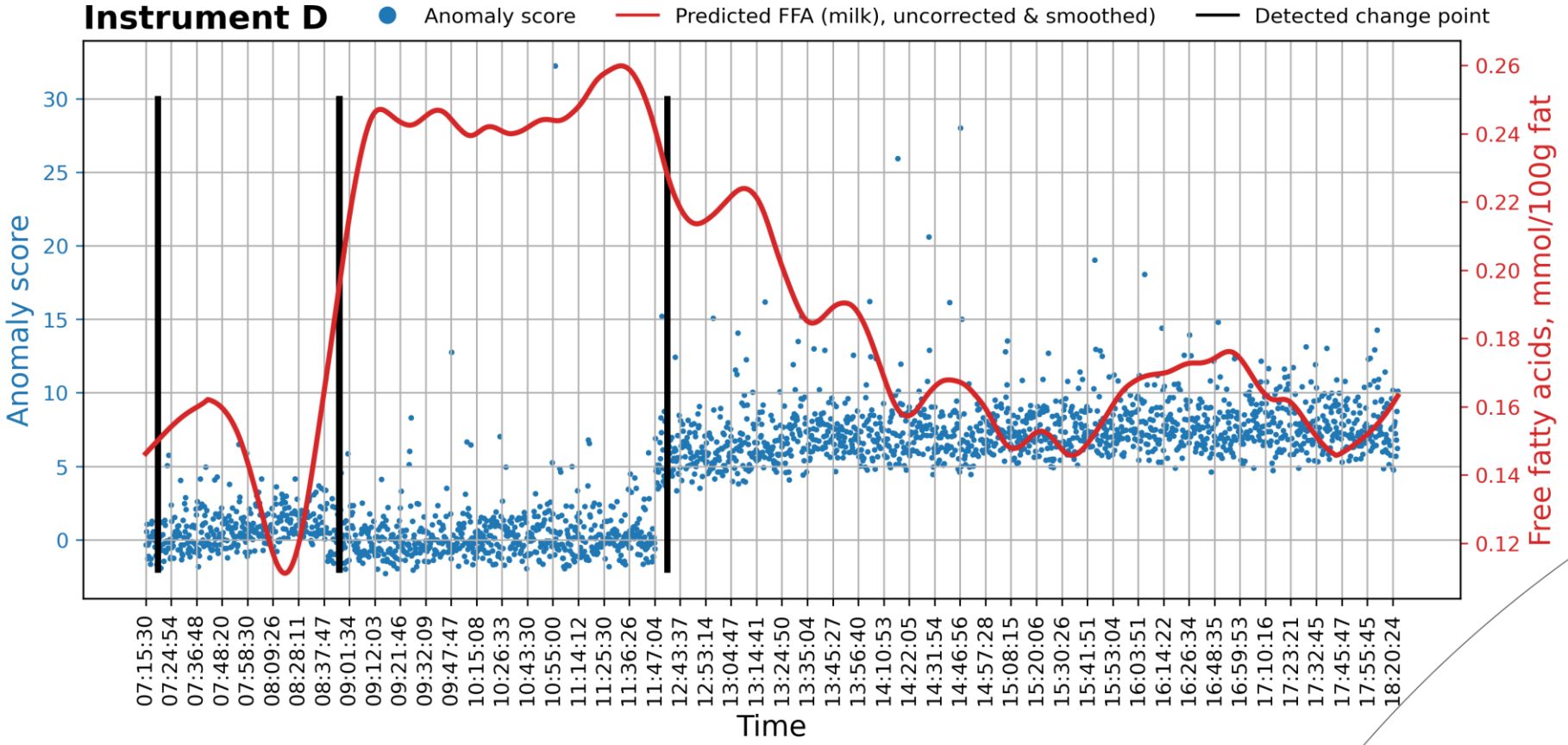

Change in anomaly scores coincides with bias in free fatty acid predictions

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Methods & Results

- Compute anomaly scores for each spectrum from the same instrument
- Look for patterns over time
- **Detect systematic deviations automatically and real-time**

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Methods & Results

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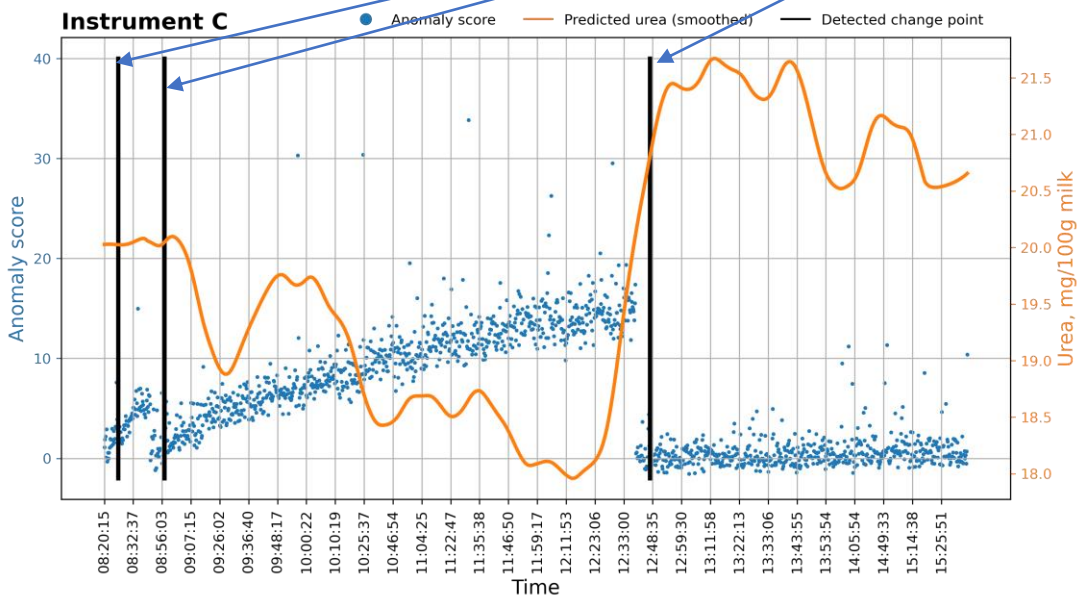
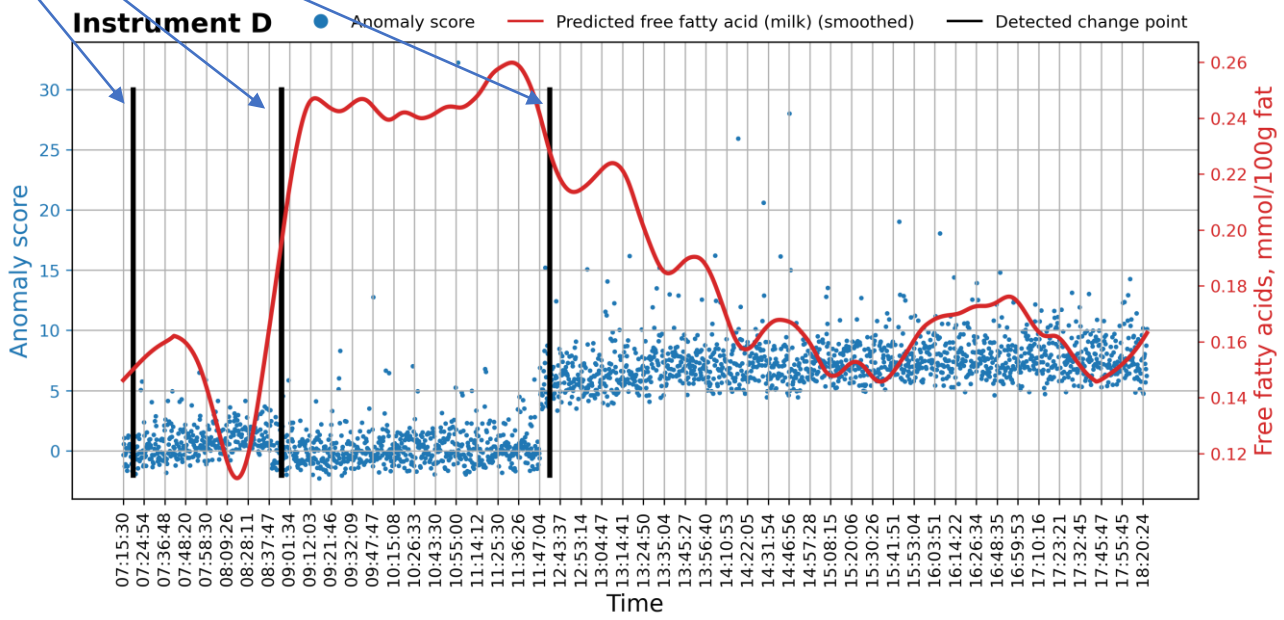
Bayesian online change point algorithm





Methods & Results

- Compute anomaly scores for each spectrum from the same instrument
- Look for patterns over time
- **On a scale of months to years**

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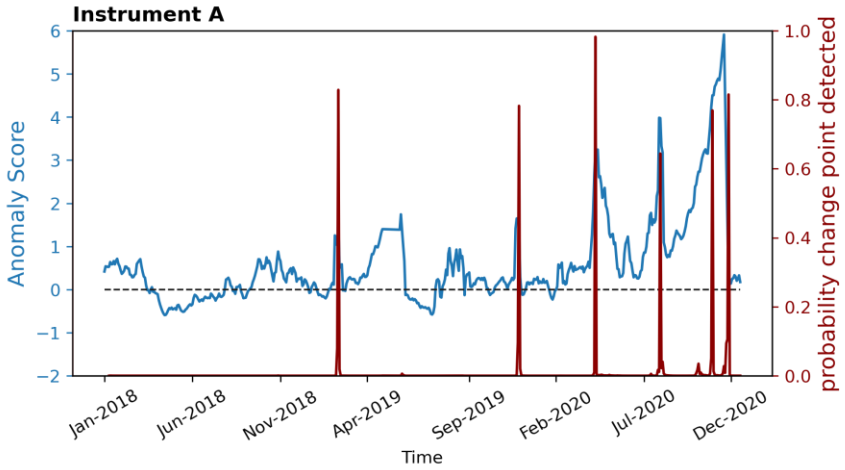

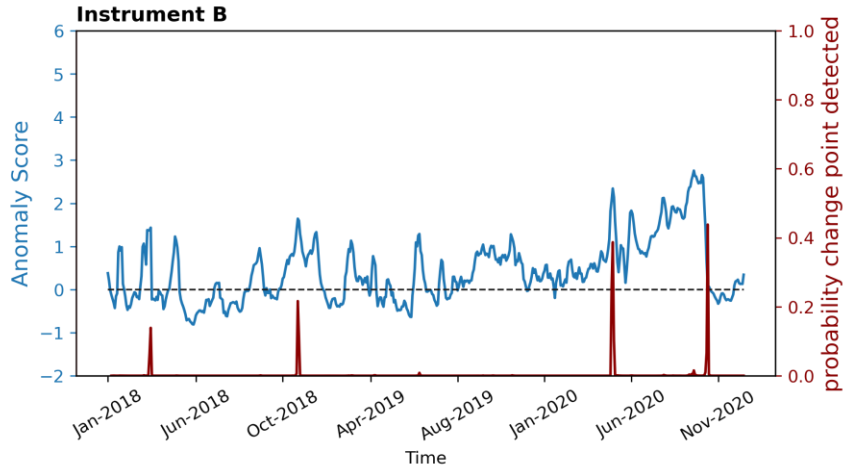

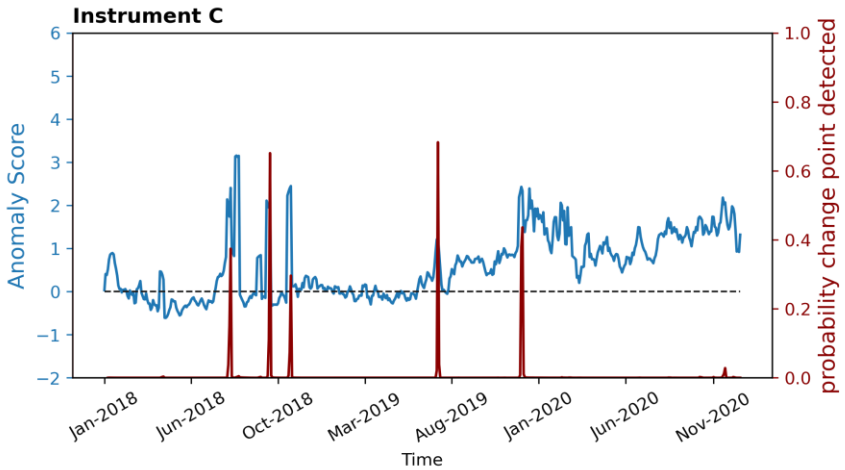

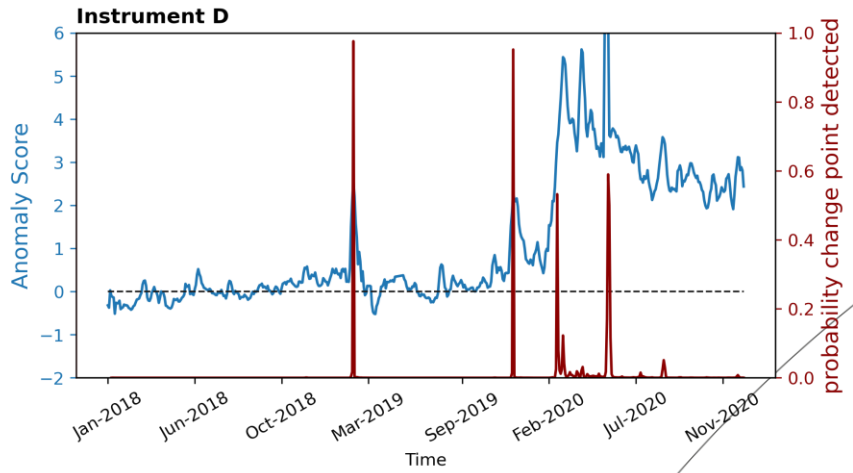

Steady drifts

&

Sudden jumps

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Methods & Results

- Compute anomaly scores for each spectrum from the same instrument
- Identify episodes with instabilities
- **Find patterns in spectral residuals**

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Collected > 20.000 spectra from 38 episodes
with instabilities identified across four instruments
within a period of three years (> 5.9 million spectra)

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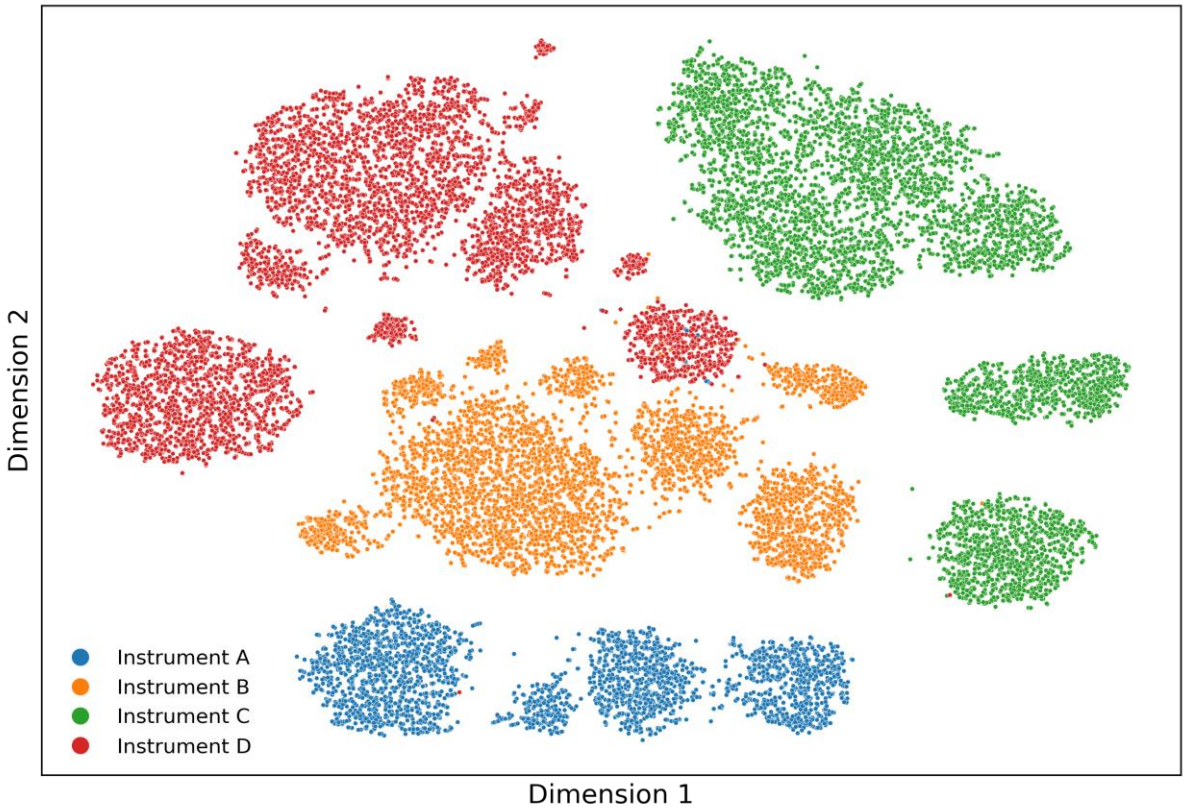
PCA + *t*-distributed stochastic neighbor embedding of spectral residuals



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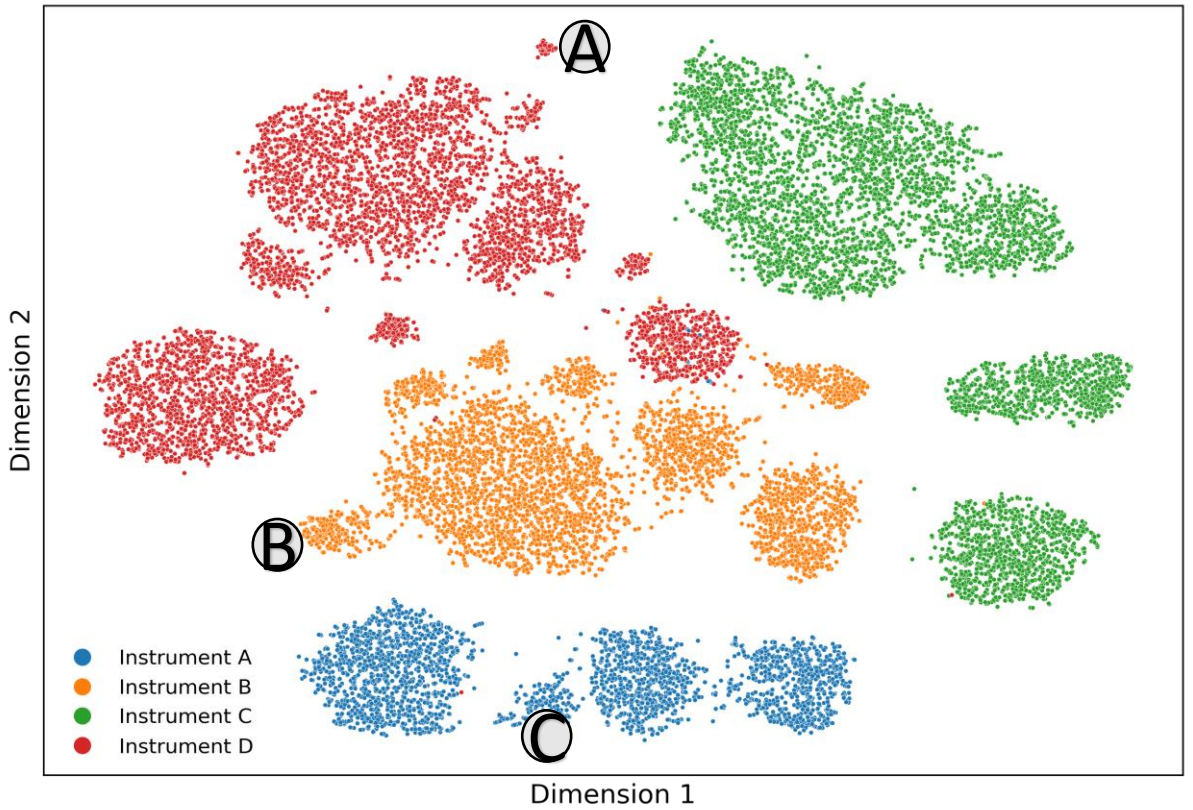
Many instabilities uniquely occur for short period Ⓐ Ⓑ Ⓒ



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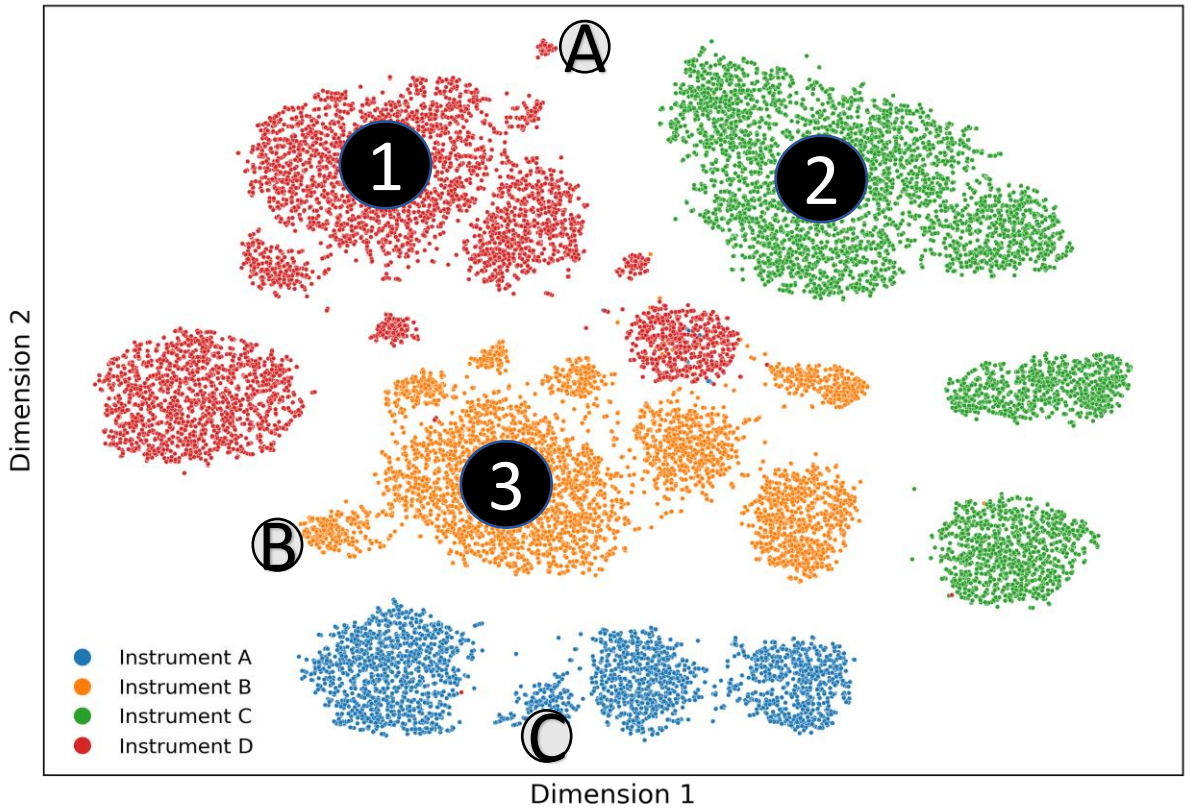
Some instabilities appear more often ❶ ❷ ❸



Summary

- Our approach can be used as tool for:
  - Monitoring the validity of our model predictions
  - Monitoring the status of our instruments
- Does not rely on expensive chemical reference analyses or control milk samples.
  - Instead, it is based on the spectra that are obtained by routine IR analysis of milk samples
- Can be developed with the tools that already exist

- Can be developed and used by every laboratory

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Thank you for your attention!

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