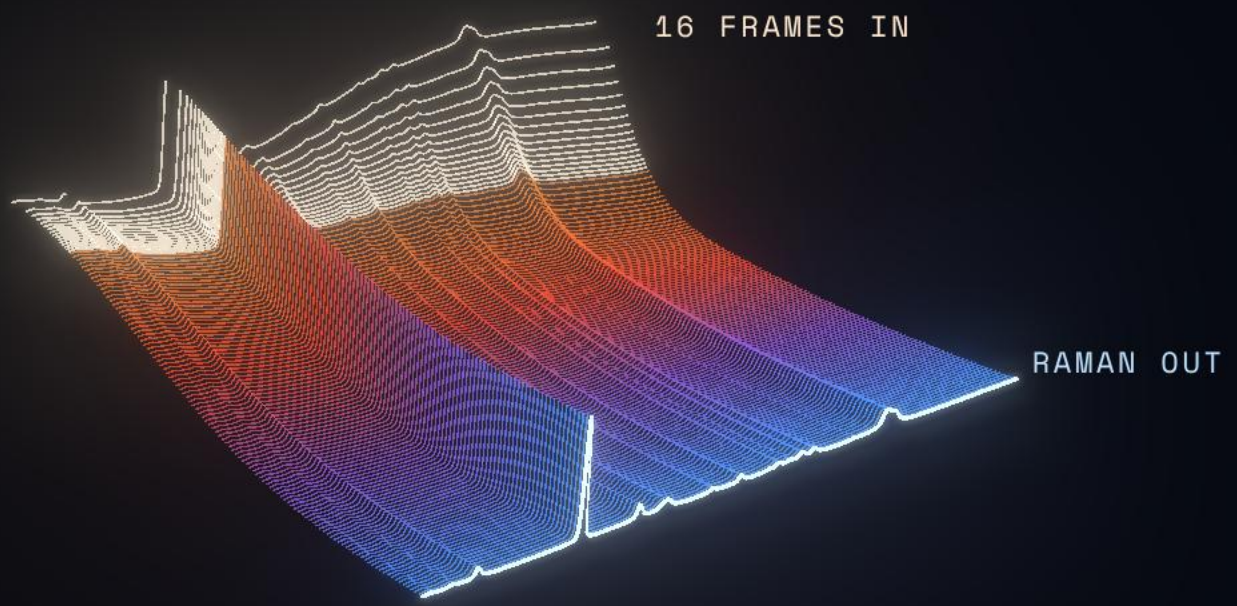
NEURIPS 2026

Unsupervised Physics Informed Decomposition of Incomplete Time-Resolved Spectroscopy

LUMOS: Latent Un-Mixing of partially Observed Spectra

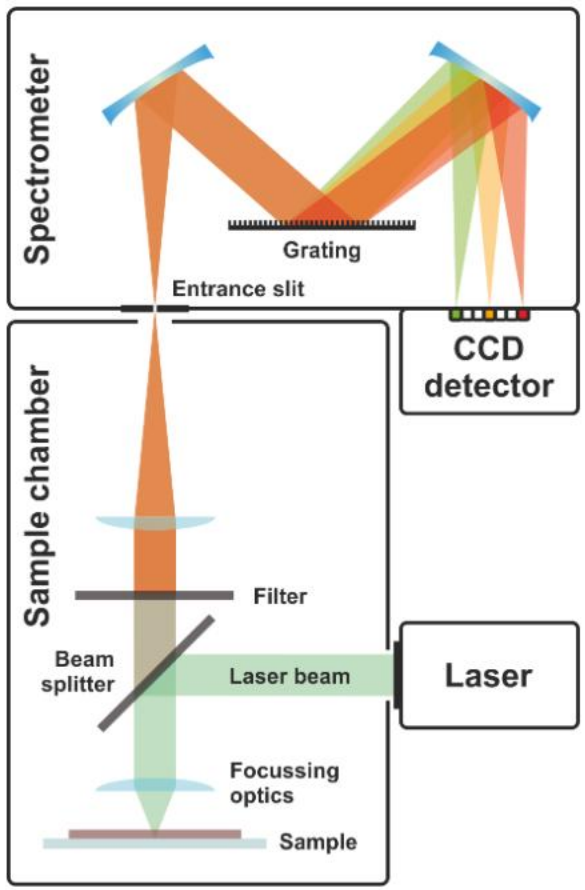
Tom Muir, Qifeng Liu, Mohammadrahim Kazemzadeh, William Mills, Aleš Leonardis, Huabing Yin, Alexander Krull

University of Birmingham · University of Glasgow



BACKGROUND

Raman spectroscopy



Instrument diagram: Schmid and Dariz, Heritage 2019, 2, 1662–1683. Detector strip and spectrum: the Raman spectrum of pharmaceutical test sample 3349; the strip is a rendering of that spectrum, not a camera image.

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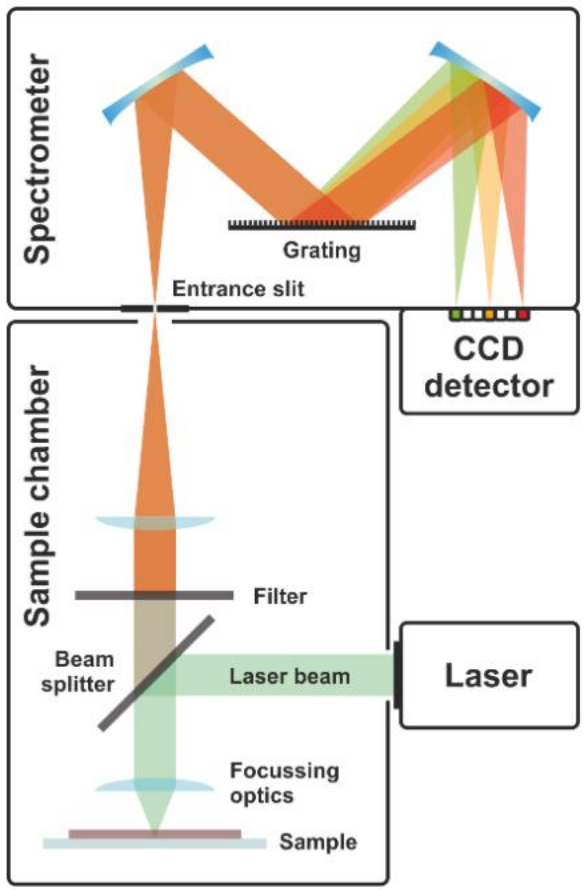



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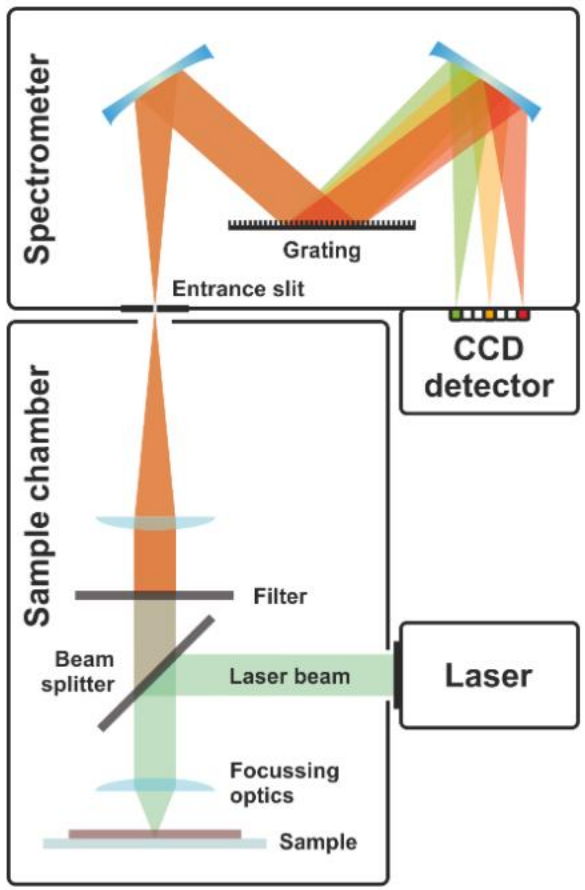

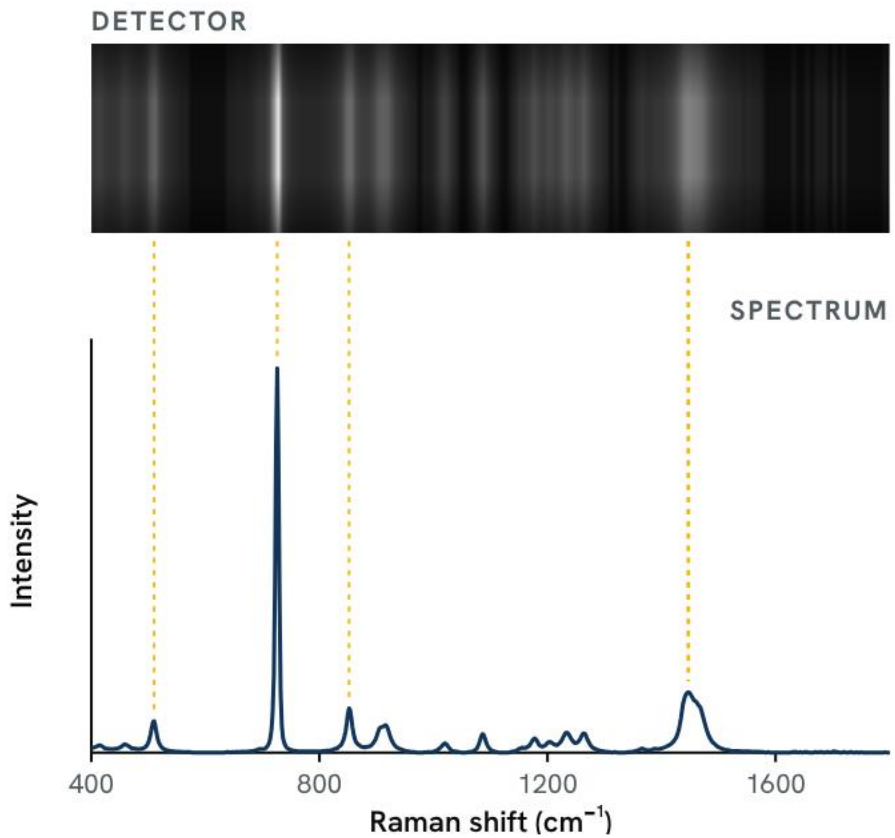

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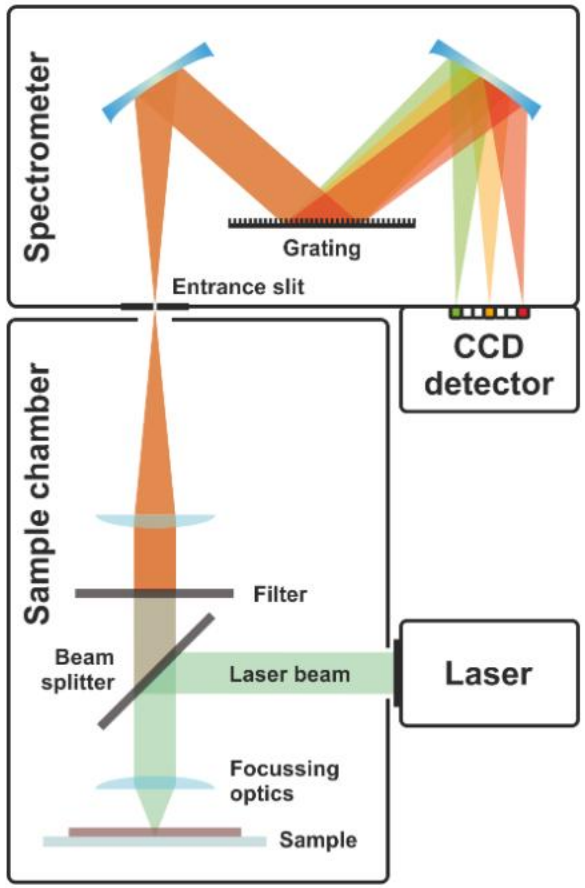

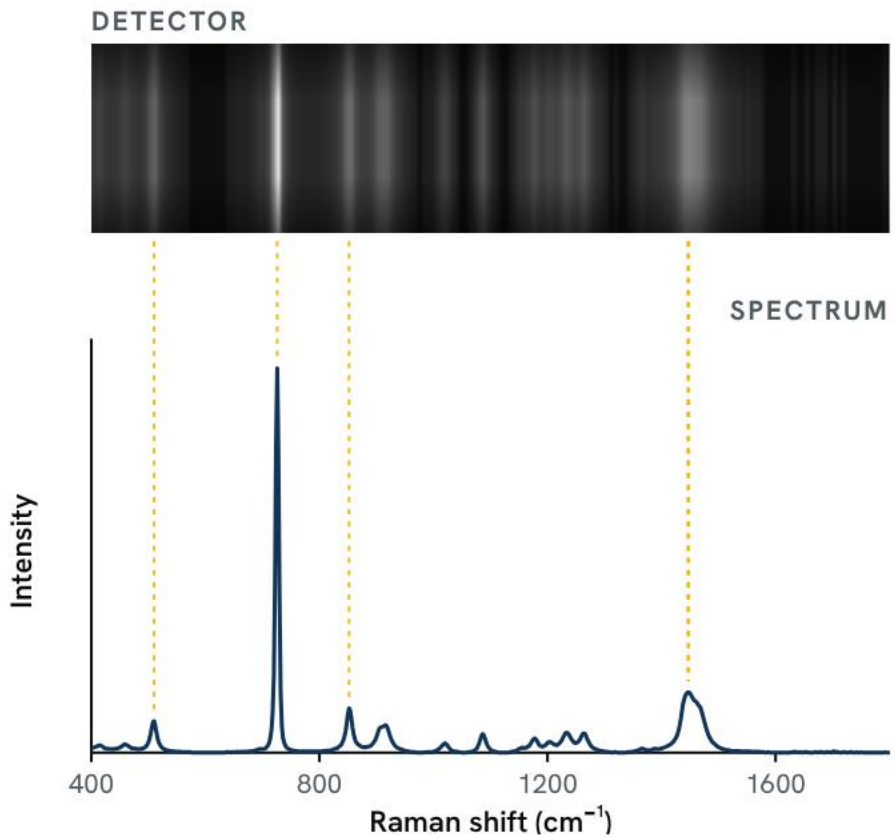

Measure and plot Raman shifts

Different molecules have unique sets of chemical bonds

The Raman spectrum acts as a biological fingerprint for the sample

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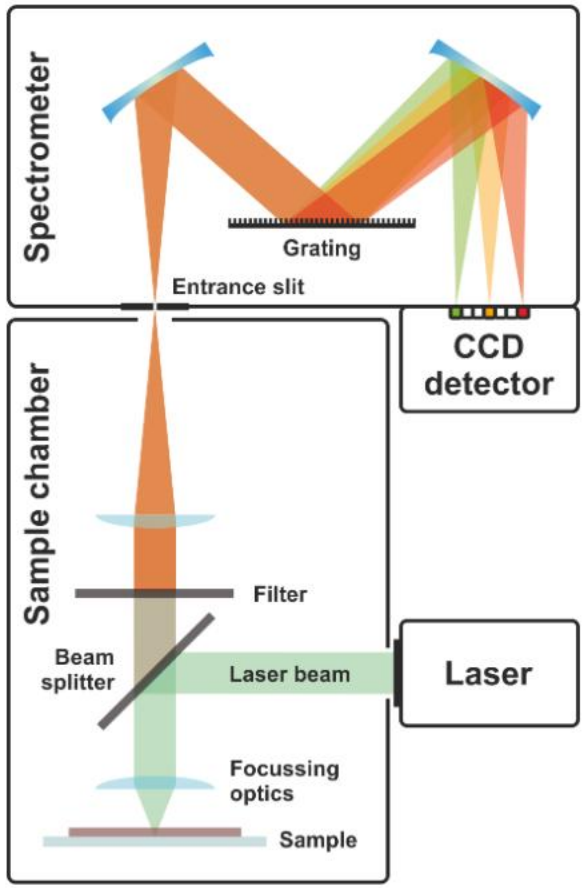

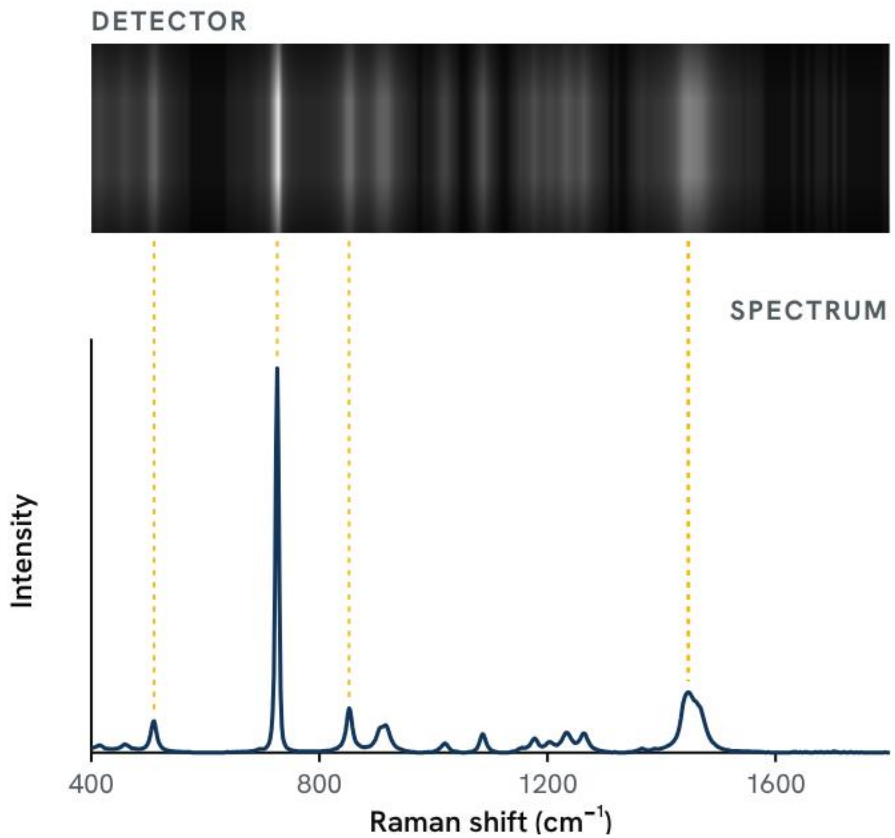

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TWO PROBLEMS

1 **Fluorescence**
A background far stronger than the Raman

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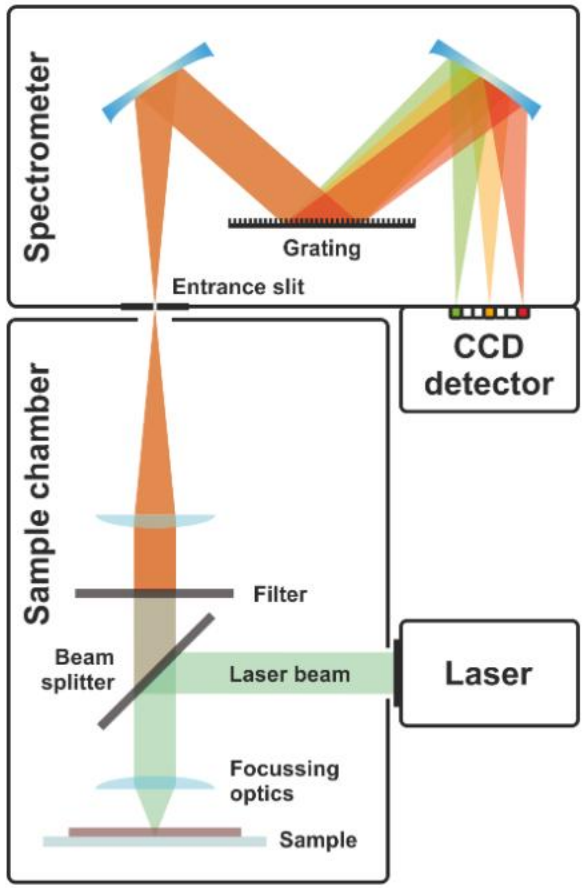

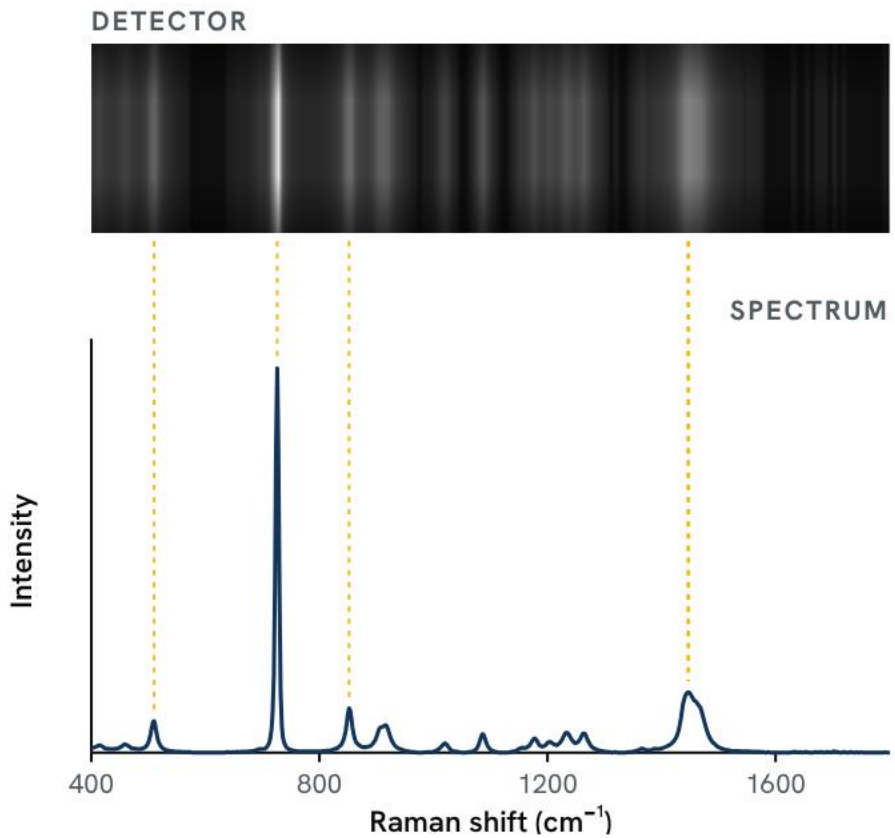

Measure and plot Raman shifts

Different molecules have unique sets of chemical bonds

The Raman spectrum acts as a biological fingerprint for the sample

TWO PROBLEMS

1 **Fluorescence**
A background far stronger than the Raman

2 **Noise**
The Raman signal is weak, so shot noise swamps it

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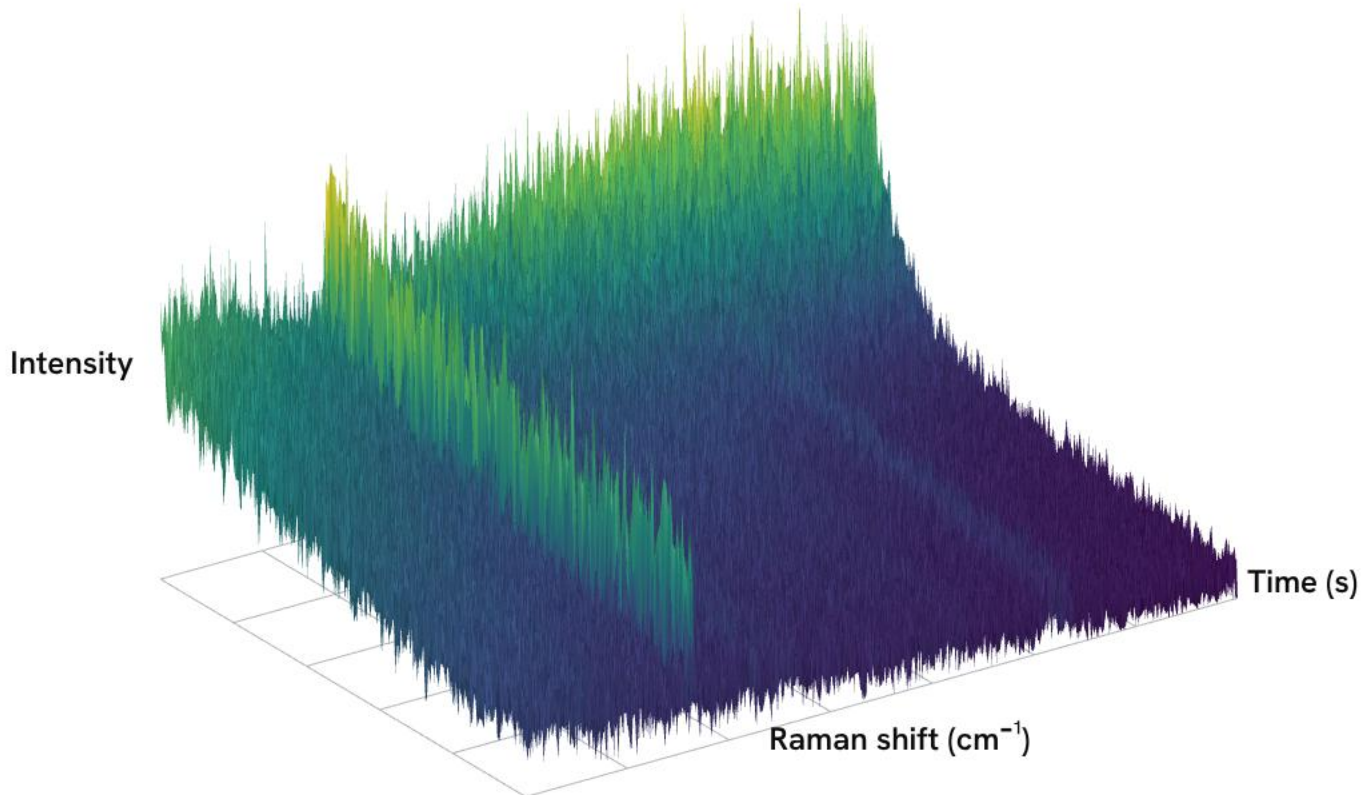
METHOD

Can we model this in full?



Pharmaceutical test sample 3349: simulated bleaching of a real Raman spectrum. The dataset holds 10 s; the last 6 s continue it with the same noise model.

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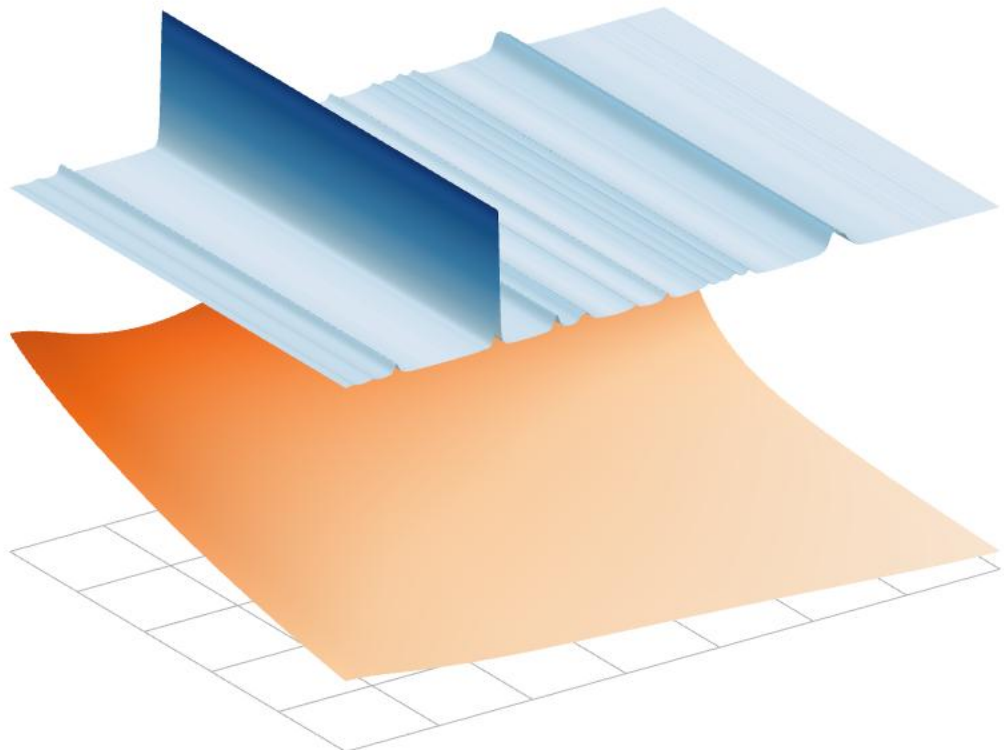

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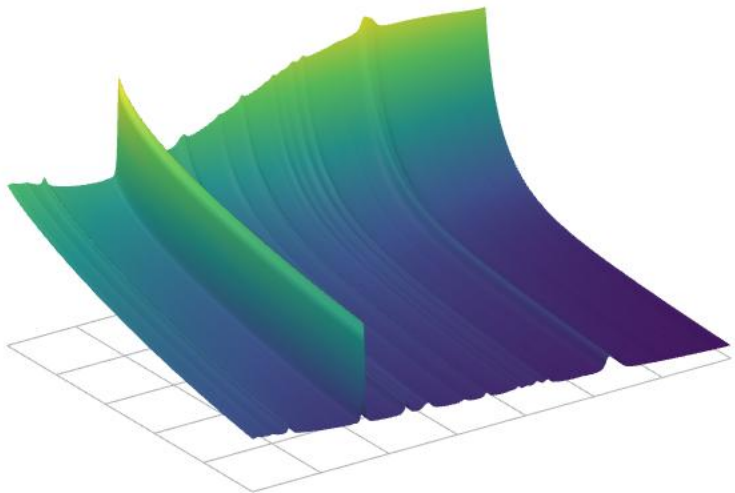
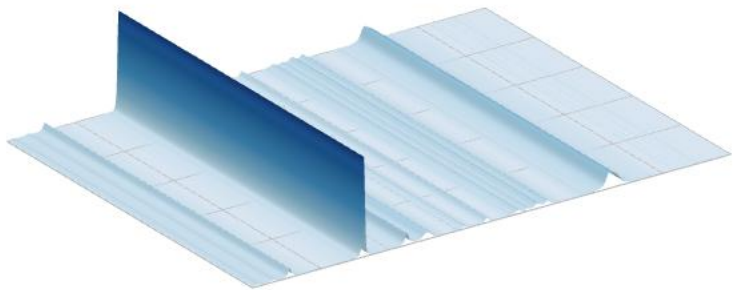
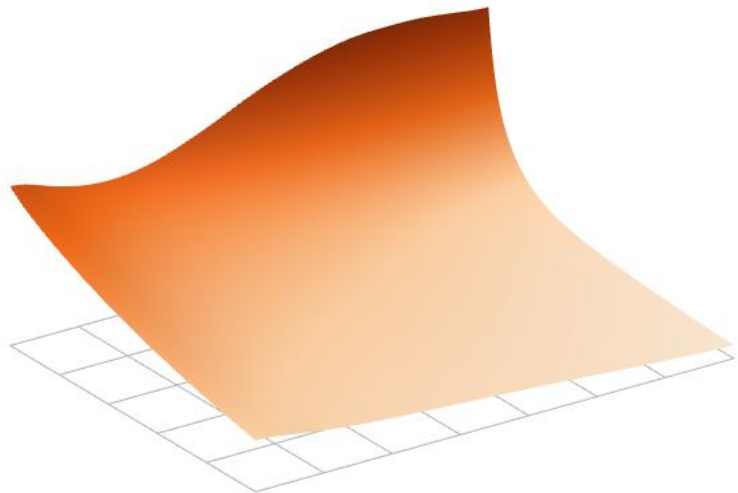


$$y(\nu, t) = \underbrace{s(\nu)}_{\text{Raman}} + \underbrace{F(\nu, t)}_{\text{Fluorescence}}$$





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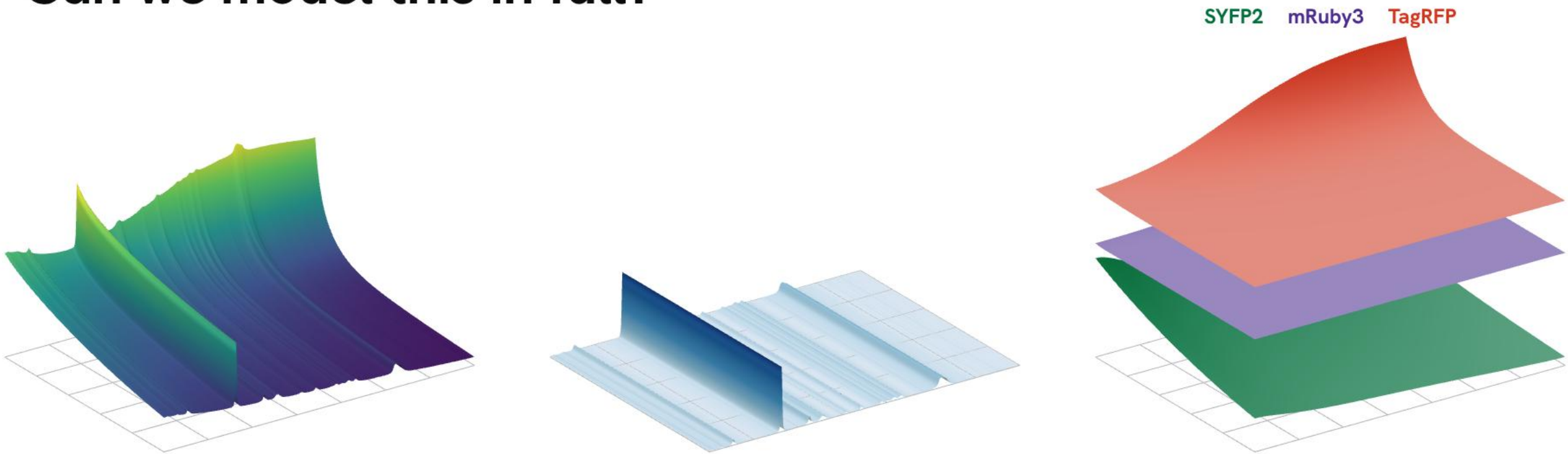

$$y(\nu,t) = \underbrace{s(\nu)}_{\text{Raman}} + \underbrace{F(\nu,t)}_{\text{Fluorescence}}$$

$$F(\nu,t) = \sum_{i=1}^{N} w_i \, B_i(\nu) \, e^{-\lambda_i t}$$

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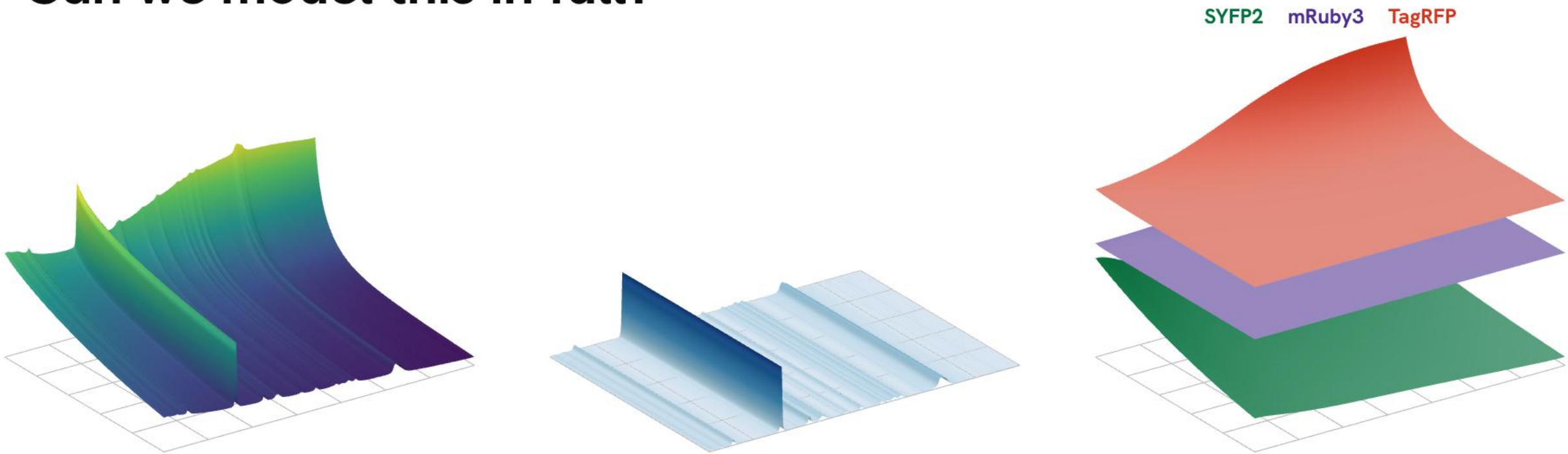

$$y(\nu, t) = \underbrace{s(\nu)}_{\text{Raman}} + \underbrace{F(\nu, t)}_{\text{Fluorescence}}$$

N : number of fluorophores

s : Raman signal (fixed)

B_i : fluorophore spectra

w_i : weight / abundance

λ_i : decay rate

$$F(\nu, t) = \sum_{i=1}^{N} w_i \, B_i(\nu) \, e^{-\lambda_i t}$$

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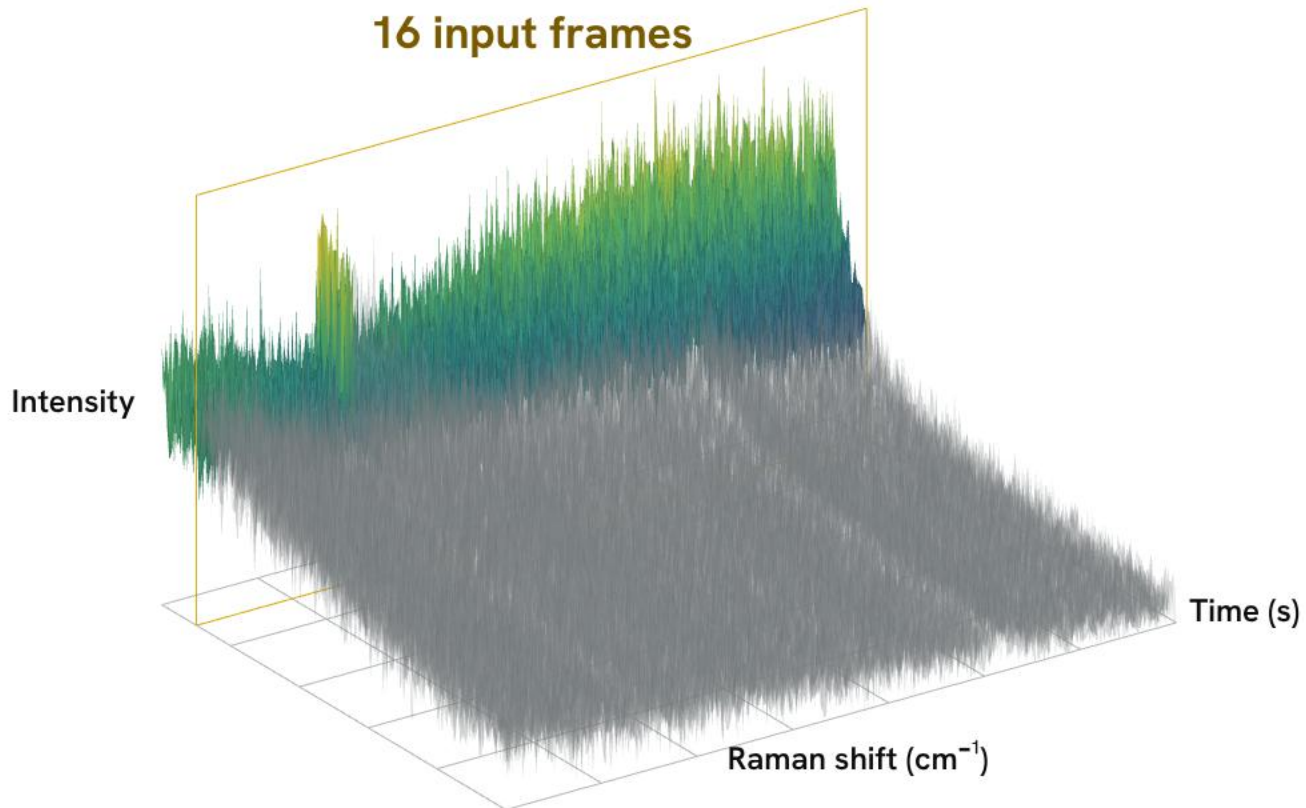

LUMOS is given only the first few frames: here 16 of 160.

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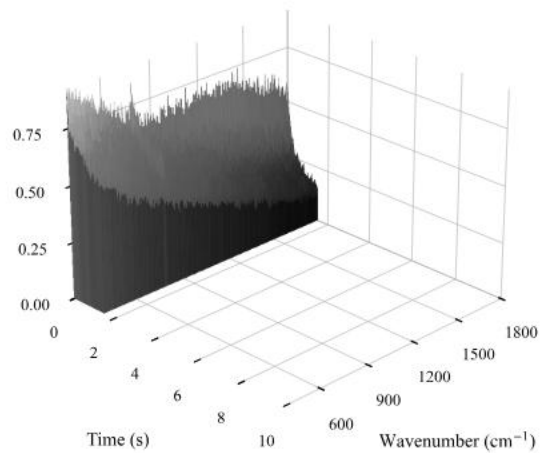
METHOD

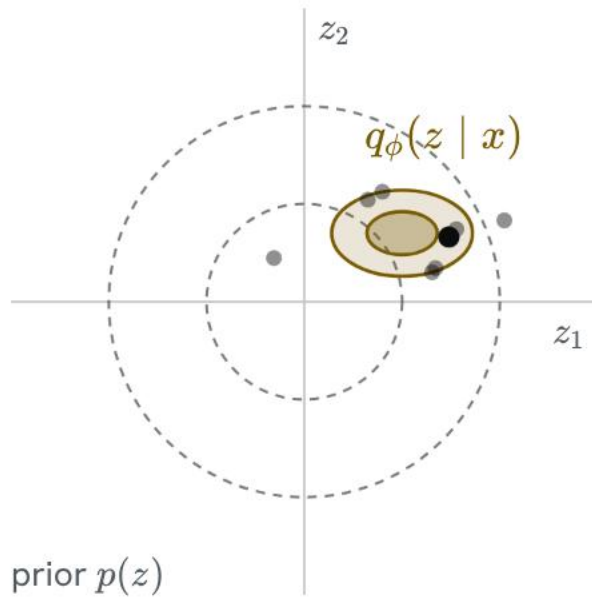
Inferring the unknowns with a VAE

Input x



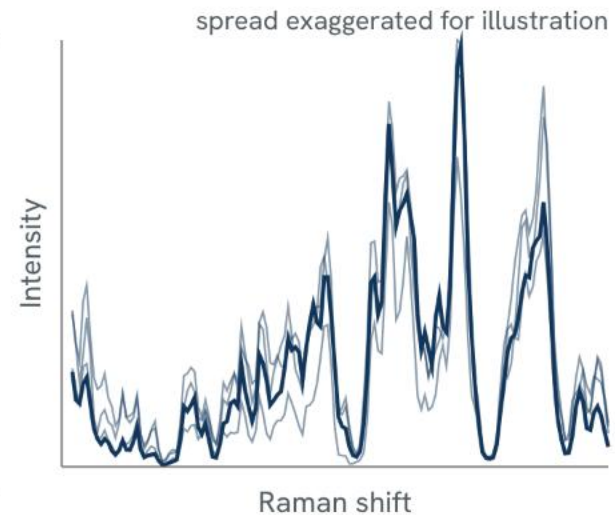
Encoder

Latent space



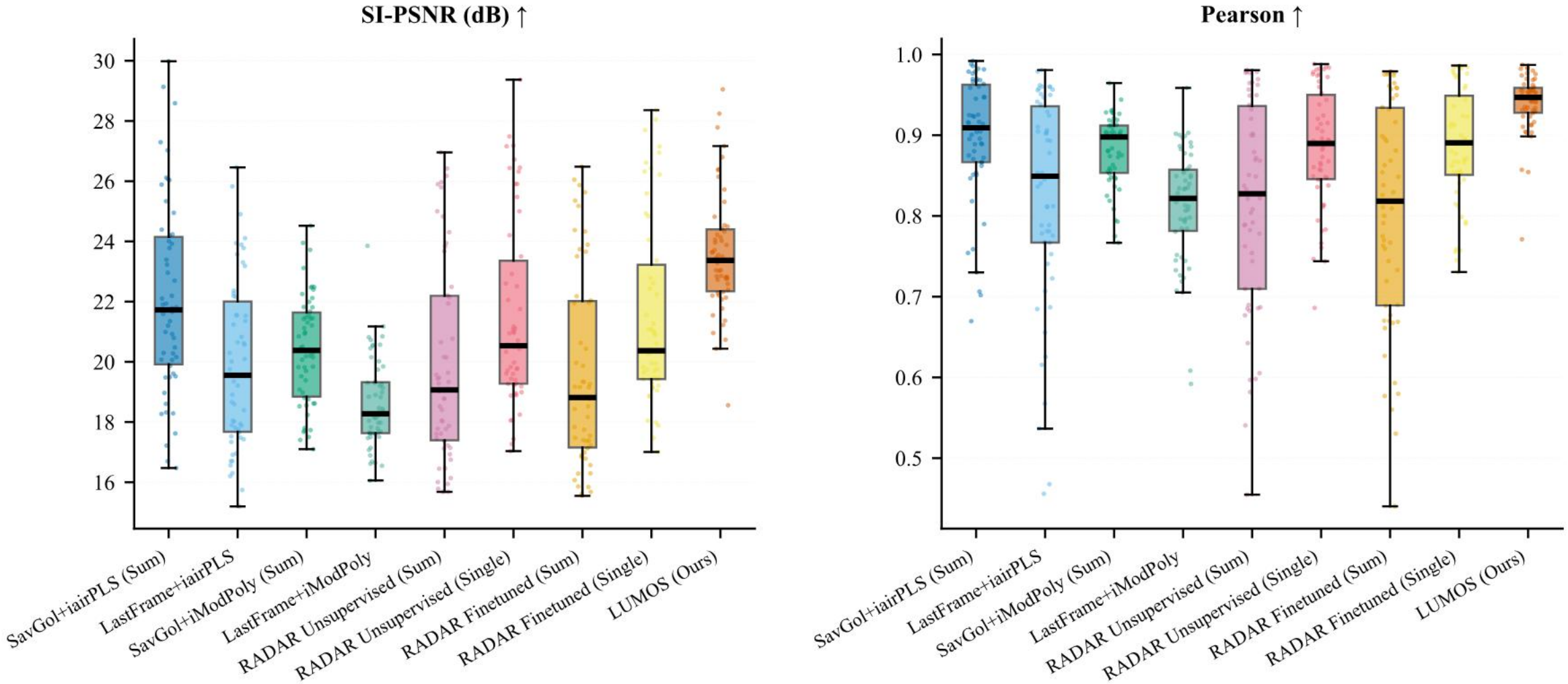
Decoder

Raman spectrum



RESULTS

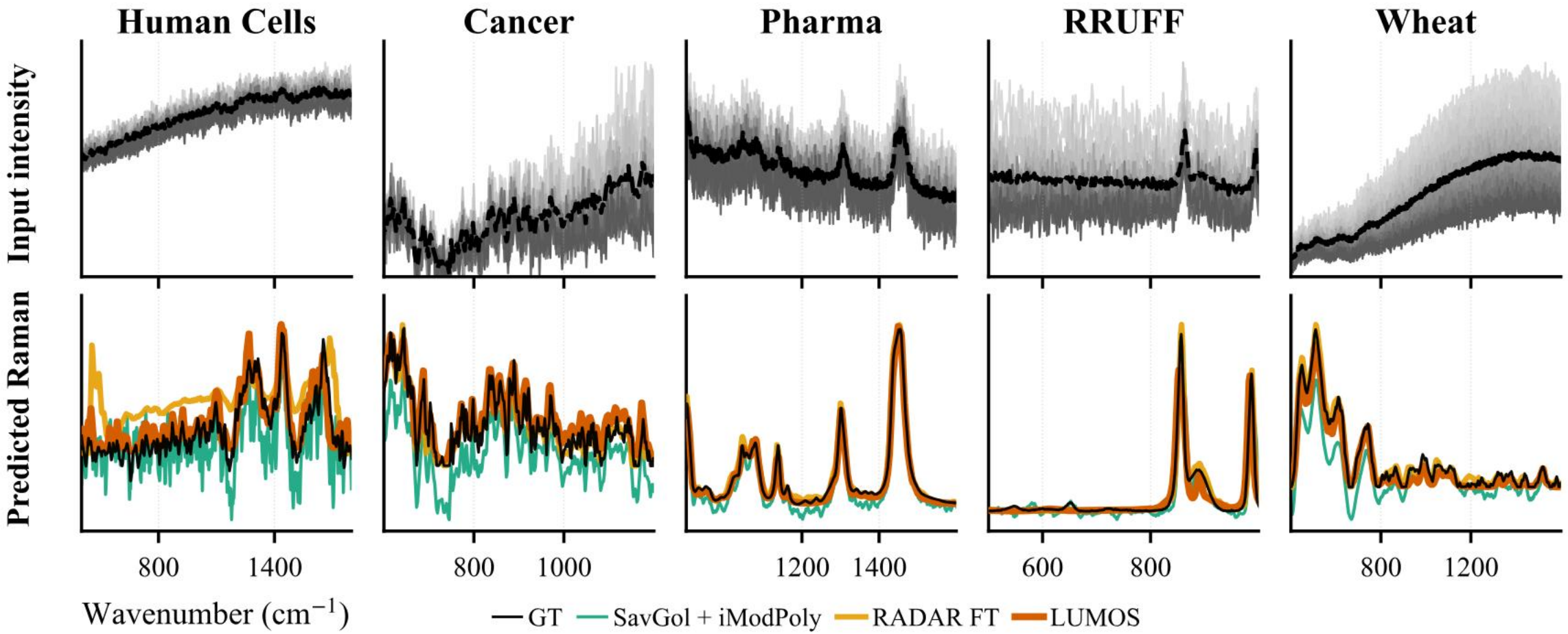
Real human cells: best and most consistent



Human cells test set (54 measured series). Each dot is one sample; boxes show the median and interquartile range. Higher is better. LUMOS never sees a clean spectrum; the fine-tuned RADAR baselines are supervised.

RESULTS

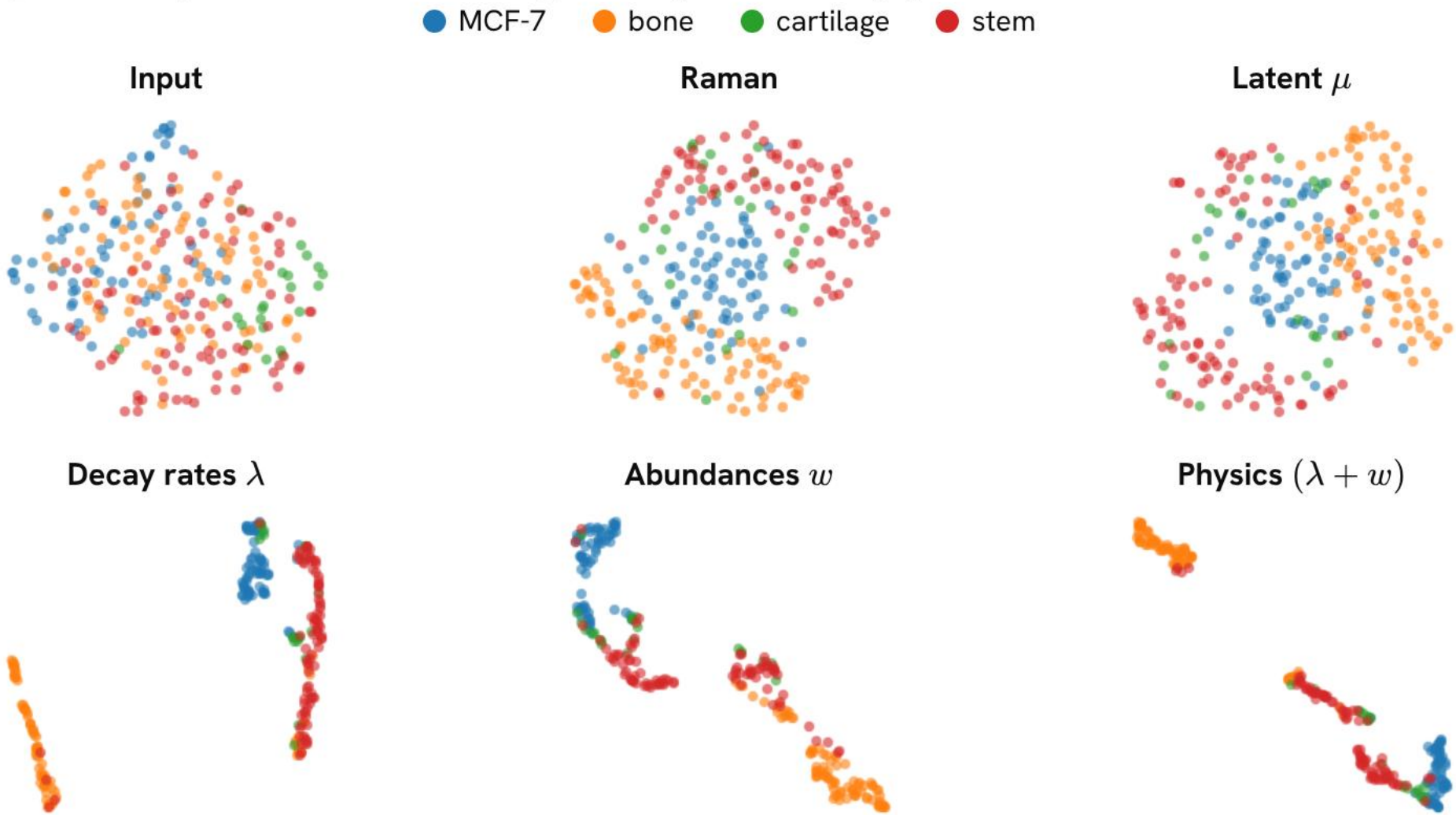
Qualitative comparison



One representative test sample per dataset. Top: the 16 input frames. Bottom: recovered Raman spectra against the ground truth (GT). Human cells are real measurements; the other four are simulated.

RESULTS

The physics parameters group cell types



UMAP (a 2D map that places similar samples close together) of each quantity LUMOS extracts from the Human cells data, coloured by cell type. MCF-7 is a breast cancer cell line.

Thank you

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CODE
github.com/krulllab/LUMOS

DATA
github.com/krulllab/LUMOS#data

POSTER Session 5 · Hall C1 · Friday