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Supplementary Materials for

Bayesian reconstruction of rapidly scanned mid-infrared optoacoustic signals enables fast, label-free chemical microscopy

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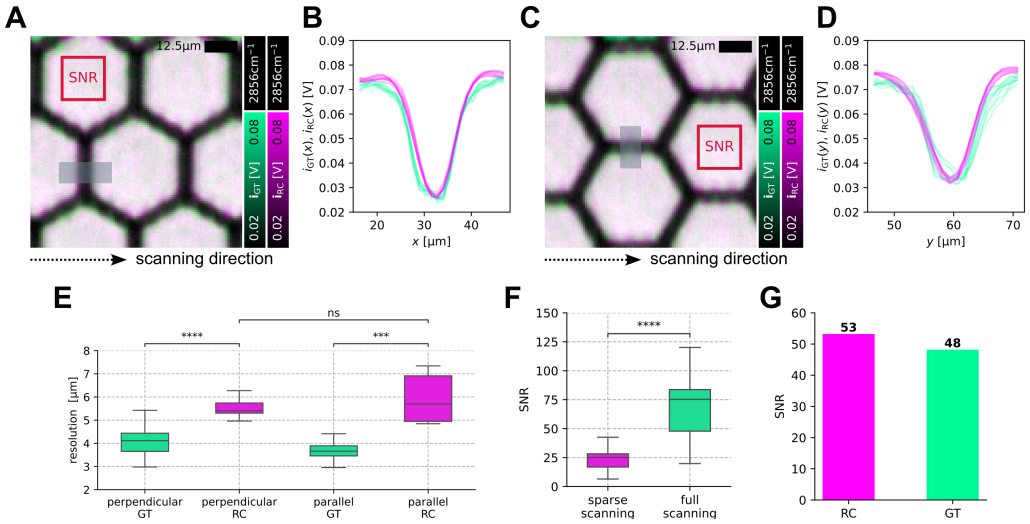
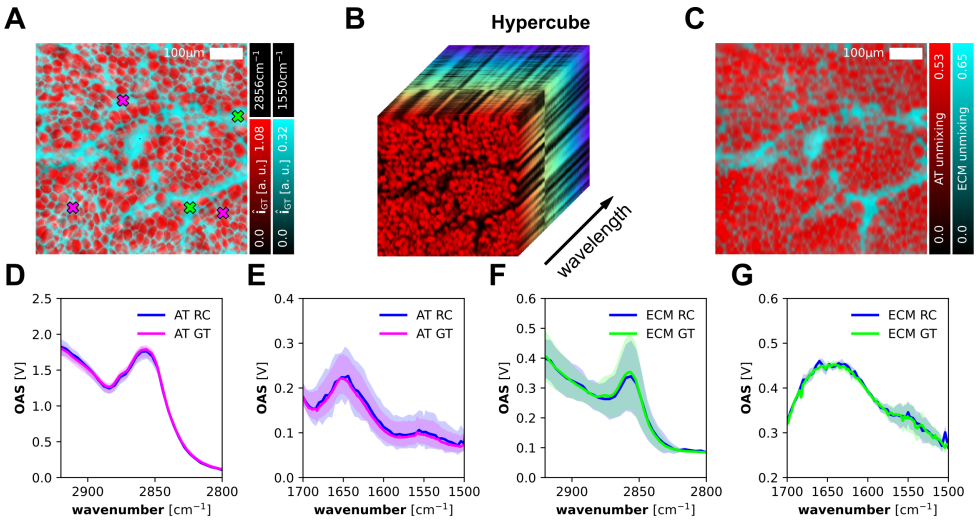
This PDF file includes:

Fig. S1.



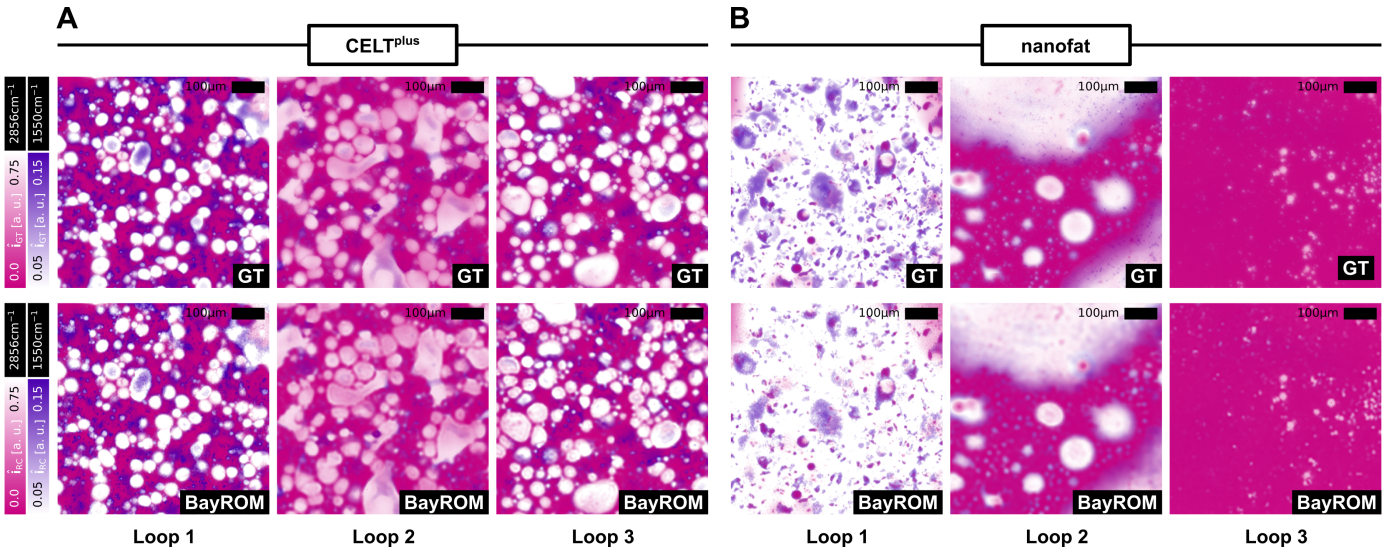
Characterization of signal-to-noise ratio (SNR) and resolution. A, Overlay of a ground truth (GT) and a BayROM image of a honeycomb phantom with sharp edges perpendicular to the scanning direction. The BayROM image was reconstructed based on down-sampled data with 92.5% data reduction. **B,** Line profiles along the scanning direction of GT (green) and reconstruction (magenta) corresponding to the images shown in **A**. **C,** Overlay of a ground truth (GT) and a BayROM image of a honeycomb phantom with sharp edges parallel to the scanning direction. The BayROM image was reconstructed based on down-sampled data with 92.5% data reduction. **D,** Line profiles along the scanning direction of GT (green) and reconstruction (magenta) corresponding to the images shown in **C**. **E,** Resolution of GT and BayROM calculated based on the edge spread functions of sharp perpendicular (GT mean: 4.0 µm; BayROM mean: 5.6 µm) and parallel edges (GT mean: 3.1 µm; BayROM mean: 4.5 µm to the scanning direction marked as grey areas in **A** and **C**. Two-sided Mann-Whitney-Wilcoxon tests were carried out to assess significance (***: $1{\cdot}10^{-4} <$ p-value $\leq 1{\cdot}10^{-3}$; ****: p-value $\leq 1{\cdot}10^{-4}$; ns: not significant). **F,** Comparison of data SNR between rapid (mean: 22.94 dB) and full scanning (mean: 67.59 dB). The data SNRs were obtained based on the optoacoustic intensities to be averaged (rapid scanning – low averaging; full scanning – high averaging) for each pixel. A two-sided Mann-Whitney-Wilcoxon test was carried out to assess significance (****: p-value $\leq 1{\cdot}10^{-4}$). **G,** Comparison of image SNR with indicated mean between BayROM (RC) and GT. The image SNR was obtained based on the intensities and their variations in the red boxes marked in **A** and **C**.

Fig. S2.



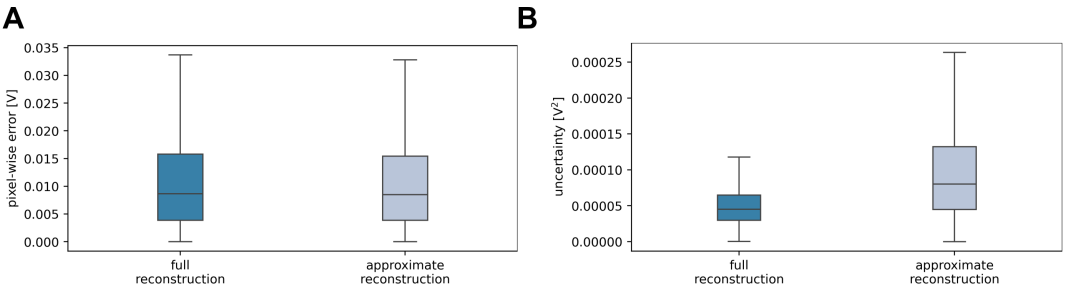
Hyperspectral adipose tissue imaging. A, White adipose tissue imaged with full raster scanning. Crosses mark selected positions representing adipocytes (AT, pink) and extracellular matrix (ECM, green). **B,** Hyperspectral BayROM image. The hypercube consisting of 80 wavenumbers was captured at the same FOV as in **A**. **C,** Pixel-wise linear unmixing of AT and ECM spectra. According to the pixel-wise unmixing coefficients, the imaged tissue consists of 66.4% adipocyte content and 33.6% ECM. **D,** Comparison of AT spectra in the lipid region. **E,** Comparison of AT spectra in the amid region. **F,** Comparison of ECM spectra in the lipid region. **G,** Comparison of ECM spectra in the amid region. The reconstructed spectra were obtained from the pixel intensities in the BayROM hypercube corresponding to the locations where the ground truth spectra were acquired. The shaded areas in **D-G** represent the ranges between the maximum and minimum spectral intensities.

Fig. S3.



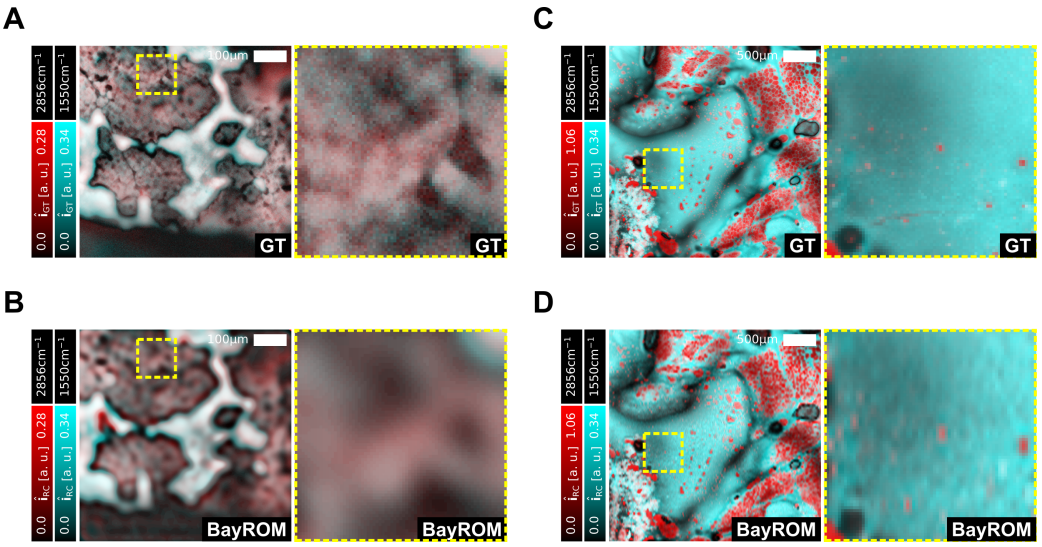
Independent measurement loops of mechanically processed fat grafts. A, Image comparisons of small field of views (FOVs), i.e., 1x1 mm^2 of Cell-Enriched Lipotransfer ($CELT^{plus}$) imaged using full raster scanning (ground truth, GT) and BayROM (92.5% data reduction). The average structural similarity index measure (SSIM), the average root mean squared error (RMSE), and the average peak signal-to-noise ratio (PSNR) between GT and BayROM are 0.90, 21.21 µV, and 23.3 dB for the scans of loop 1, respectively. The average SSIM, the average RMSE, and the average PSNR between GT and BayROM are 0.91, 13.27 µV, and 31.0 dB for the scans of loop 2, respectively. The average SSIM, the average RMSE, and the average PSNR between GT and BayROM are 0.91, 17.9 µV, and 30.37 dB for the scans of loop 3, respectively. **B,** Image comparisons of small FOVs, i.e., 1x1 mm^2 of nanofat imaged using full raster scanning (GT) and BayROM (92.5% data reduction). The average SSIM, the average RMSE, and the average PSNR between GT and BayROM are 0.78, 17.4 µV, and 26.49 dB for the scans of loop 1, respectively. The average SSIM, the average RMSE, and the average PSNR between GT and BayROM are 0.85, 11.25 µV, and 32.62 dB for the scans of loop 2, respectively. The average SSIM, the average RMSE, and the average PSNR between GT and BayROM are 0.87, 9.76 µV, and 29.83 dB for the scans of loop 3, respectively.

Fig. S4.



Comparison between full and approximate reconstruction. A, Comparison of pixel-wise error for full and approximate reconstruction. **B,** Comparison of pixel-wise uncertainty for full and approximate reconstruction. An approximate result can be obtained to speed up the reconstruction process by reducing computational complexity. Reconstruction based on 5 iterations of metric Gaussian variational inference (MGVI) and 16 samples drawn from the posterior distribution are considered full reconstructions, while approximate reconstructions were carried out using 3 iterations of MGVI and 8 samples drawn from the posterior distribution. The approximation (obtained in 2 min 38 s) has a similar error distribution as the full reconstruction (obtained in 10 min 6 s). However, the approximate reconstruction comes with less confidence (higher uncertainty) compared to the full reconstruction.

Fig. S5.



Blur and noisy artifacts. A-B, Ground truth (GT) hyperspectral image and BayROM hyperspectral image (92.5% sparsity) of mouse liver tissue demonstrating a blur artifact. The average root mean squared error (RMSE) and the average peak signal-to-noise ratio (PSNR) between GT and BayROM are 6.886 µV and 28.28 dB. **C-D,** Ground truth (GT) hyperspectral image and BayROM hyperspectral image (92.5% sparsity) of pancreatic mouse tissue demonstrating a noisy artifact. The average RMSE and the average PSNR between GT and BayROM are 15.79 µV and 33.02 dB for the small FOVs.