

Signal Conditioning and Filtering of SELDI MS Time Series

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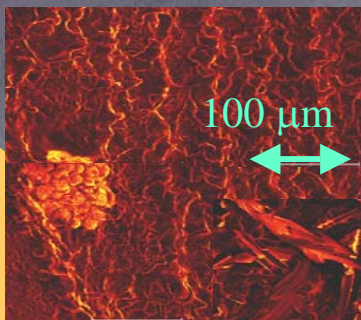


new data

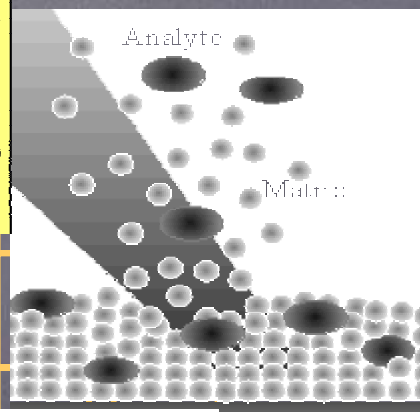
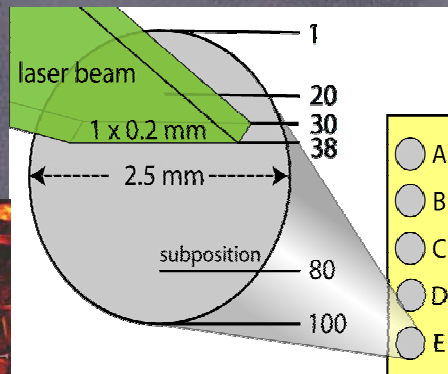
familiar problems

known techniques

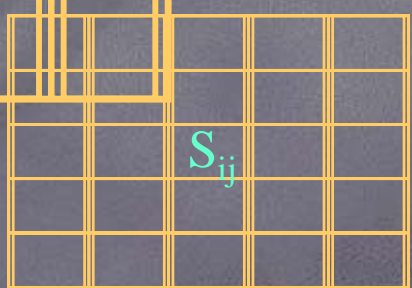
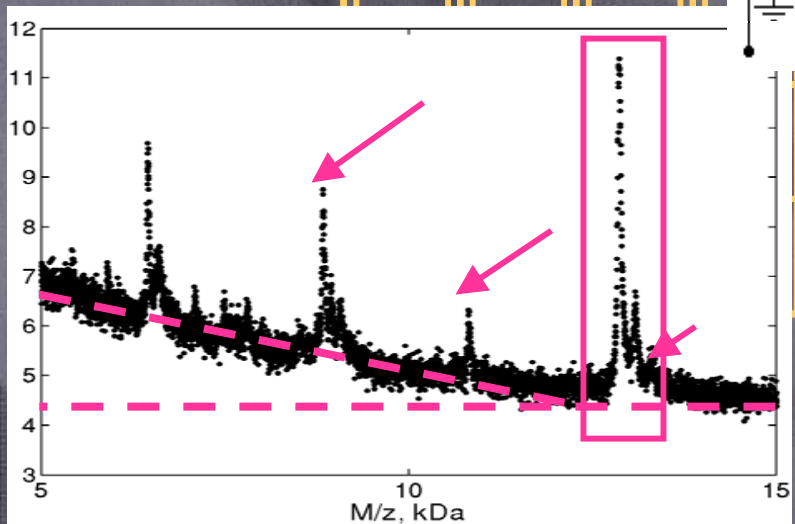
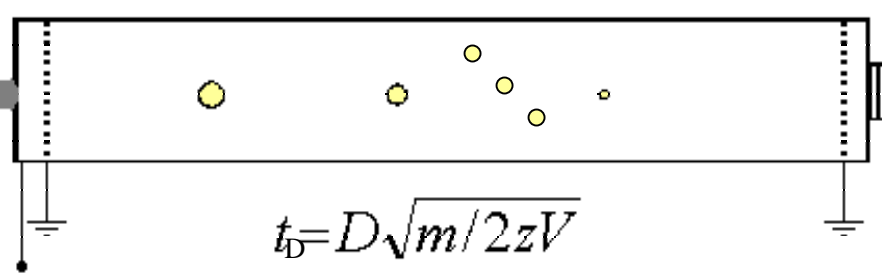
SELDI Profiling: Sources of Error



100 μm

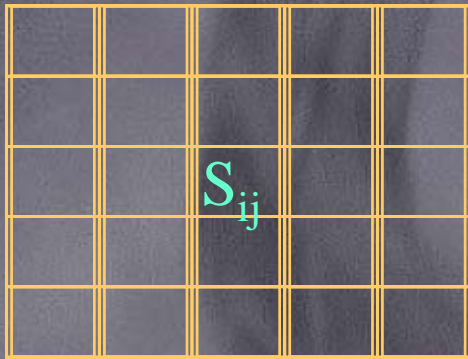


LONG WAY!



Signal Conditioning Issues

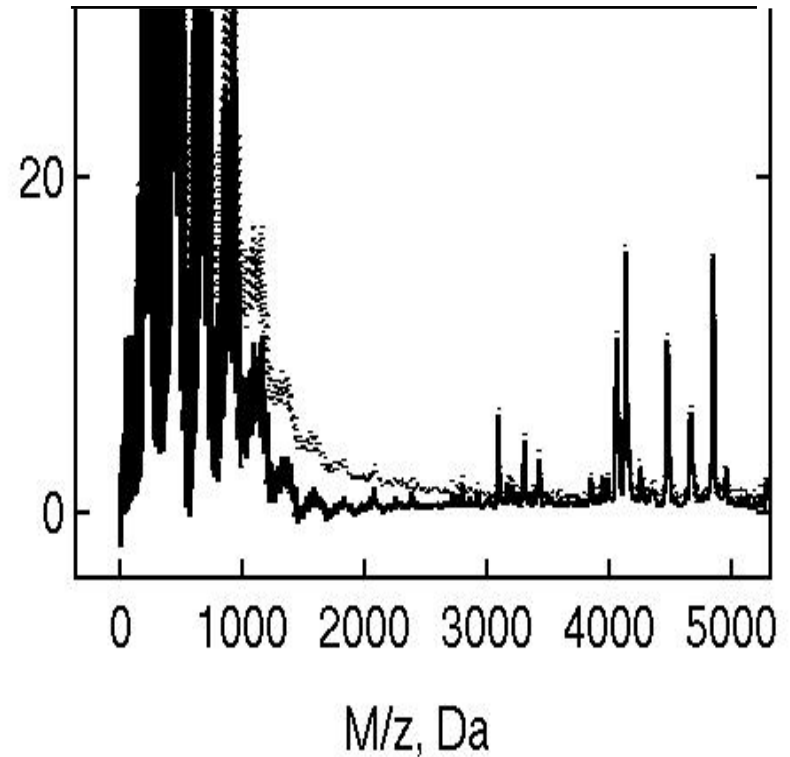
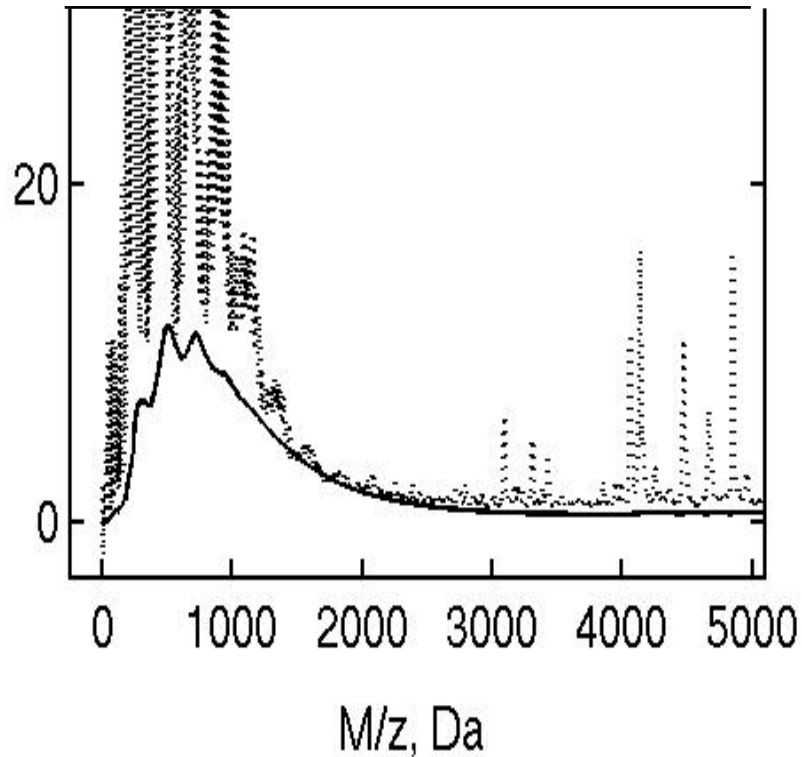
- Peak relevance: biological or artifact?
 - noise characterization
- Peak location: which column entry?
 - deconvolution filtering
- Peak intensity: which value entry?
 - background removal



		S_{ij}		

Baseline Correction

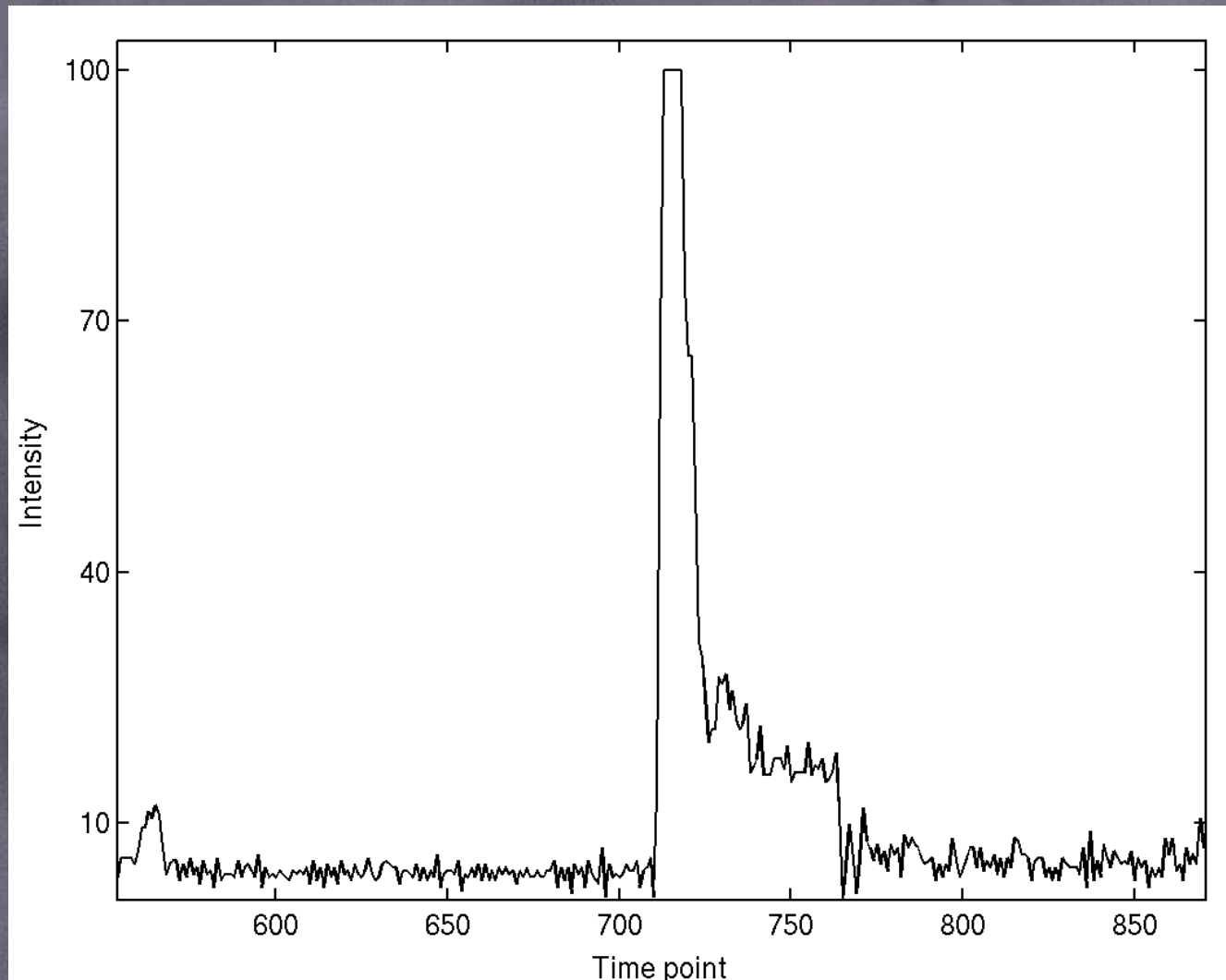
Peak intensity in the data matrix



- Baseline is predictable from RC modeling
- Single shot or average data

Nonlinear Baseline

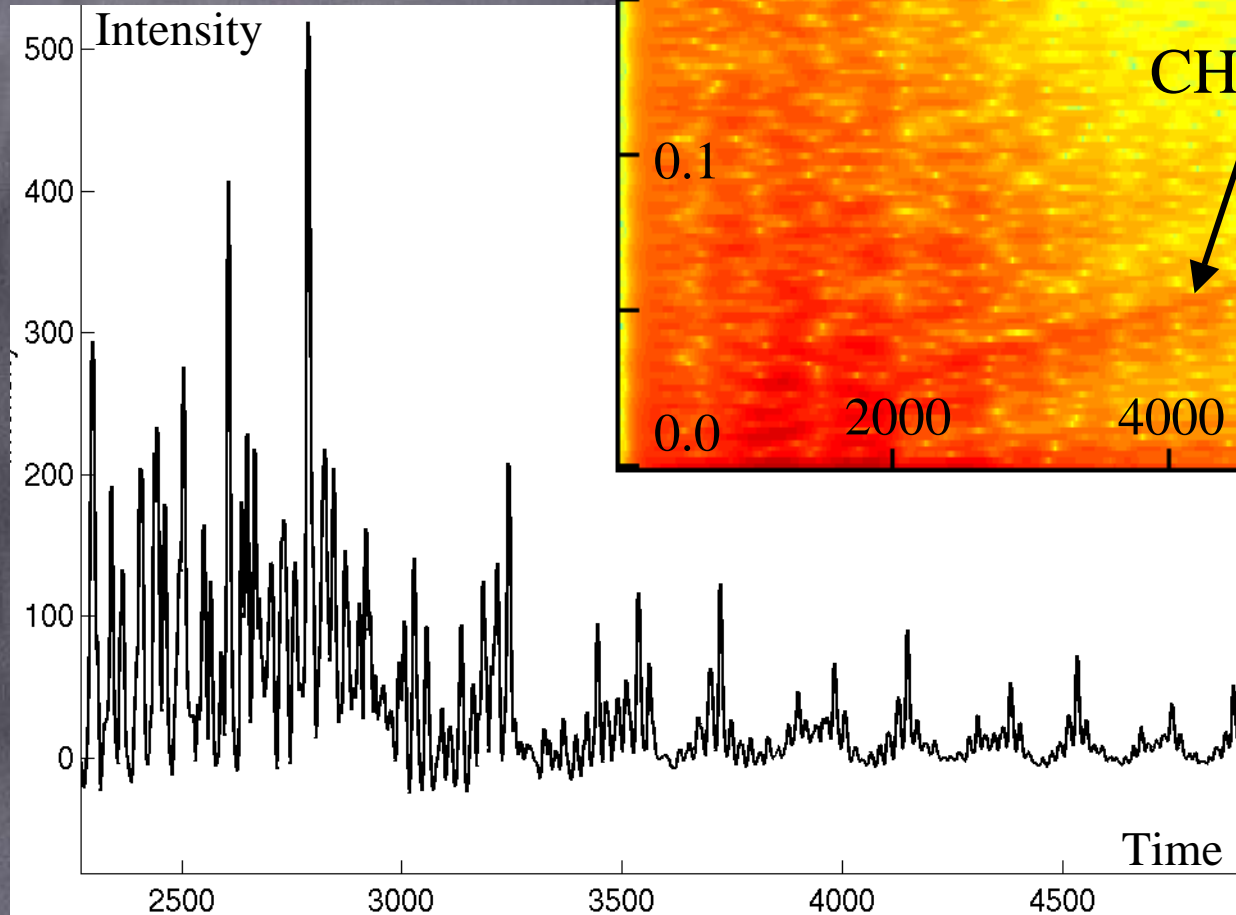
Peak intensity and biological relevance



- Length is proportional to the number of overload points
- Single shot correction **only**

Baseline Ringing

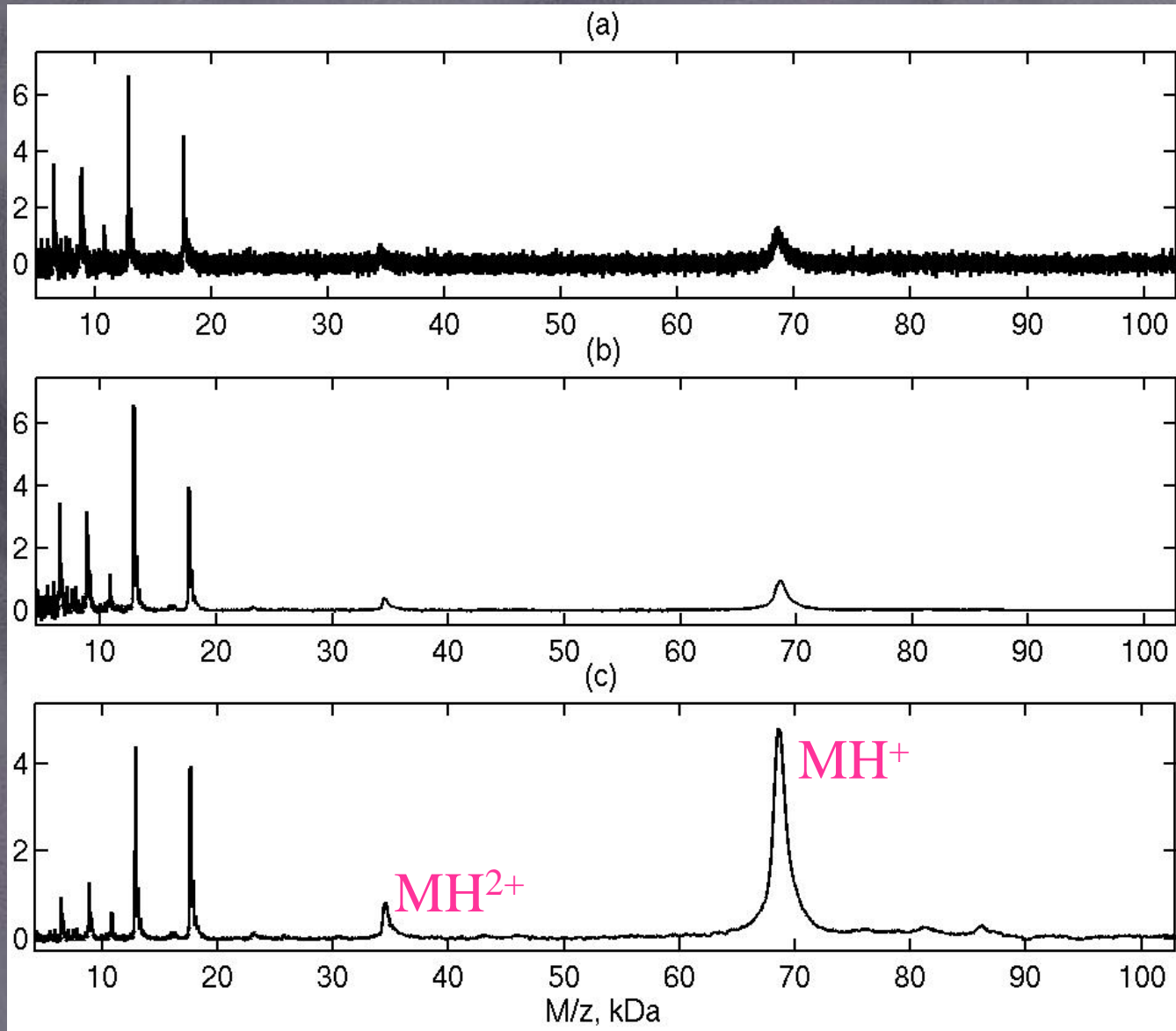
Peak relevance



- Damped coherent oscillation after overload
- Should be subtracted after each single shot

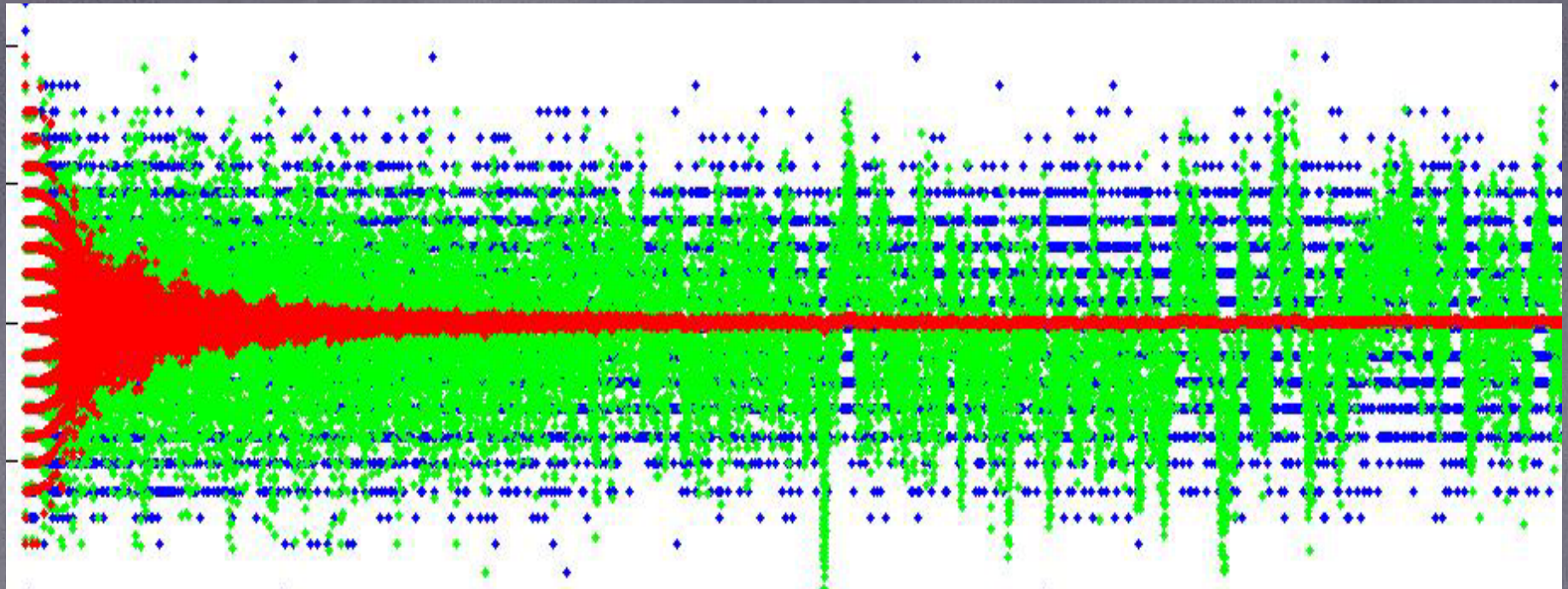
Smoothing & Rescaling

Peak relevance and intensity



Rescaling & Noise

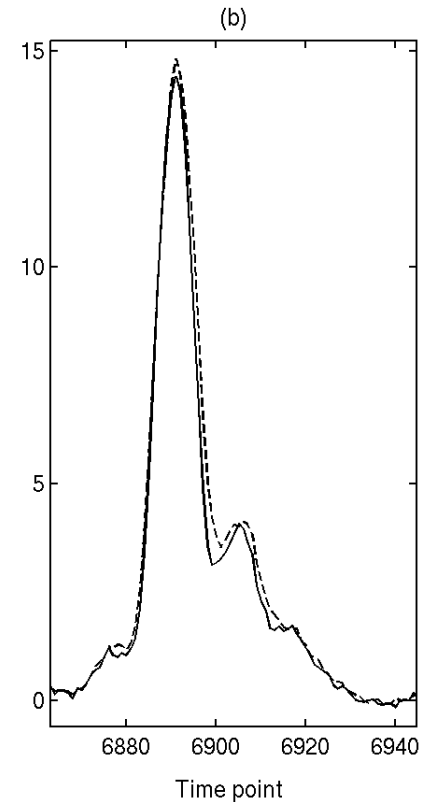
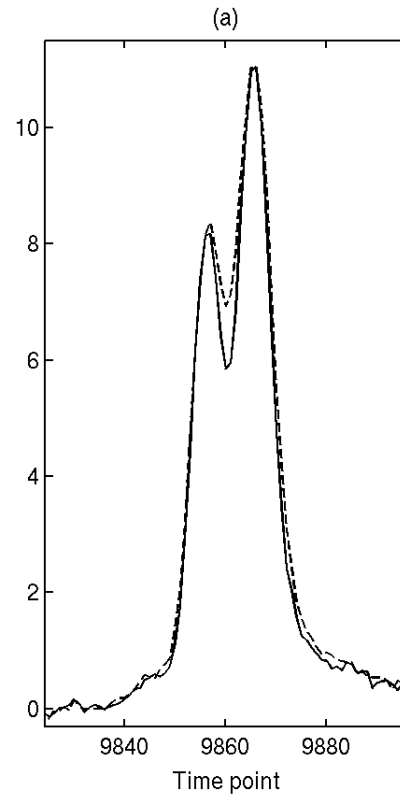
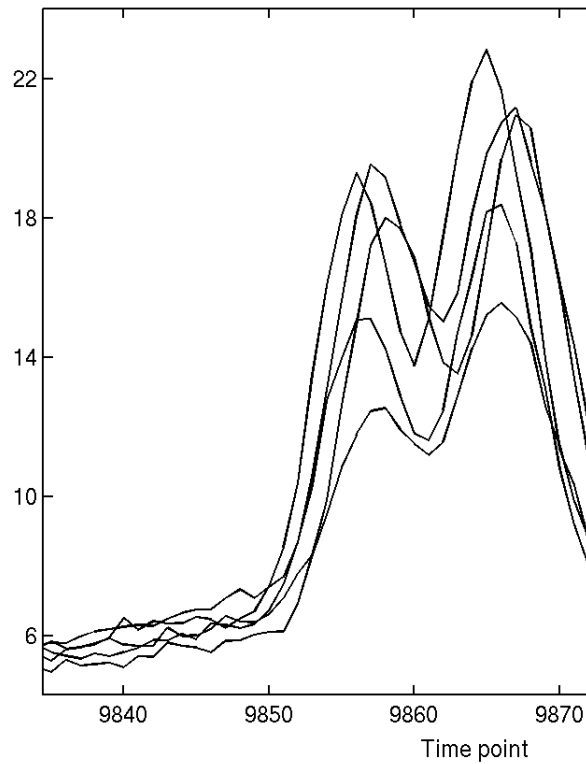
Peak relevance



- Provides constant noise amplitude
- Filtered noise is “colored”

Subposition De-Jittering

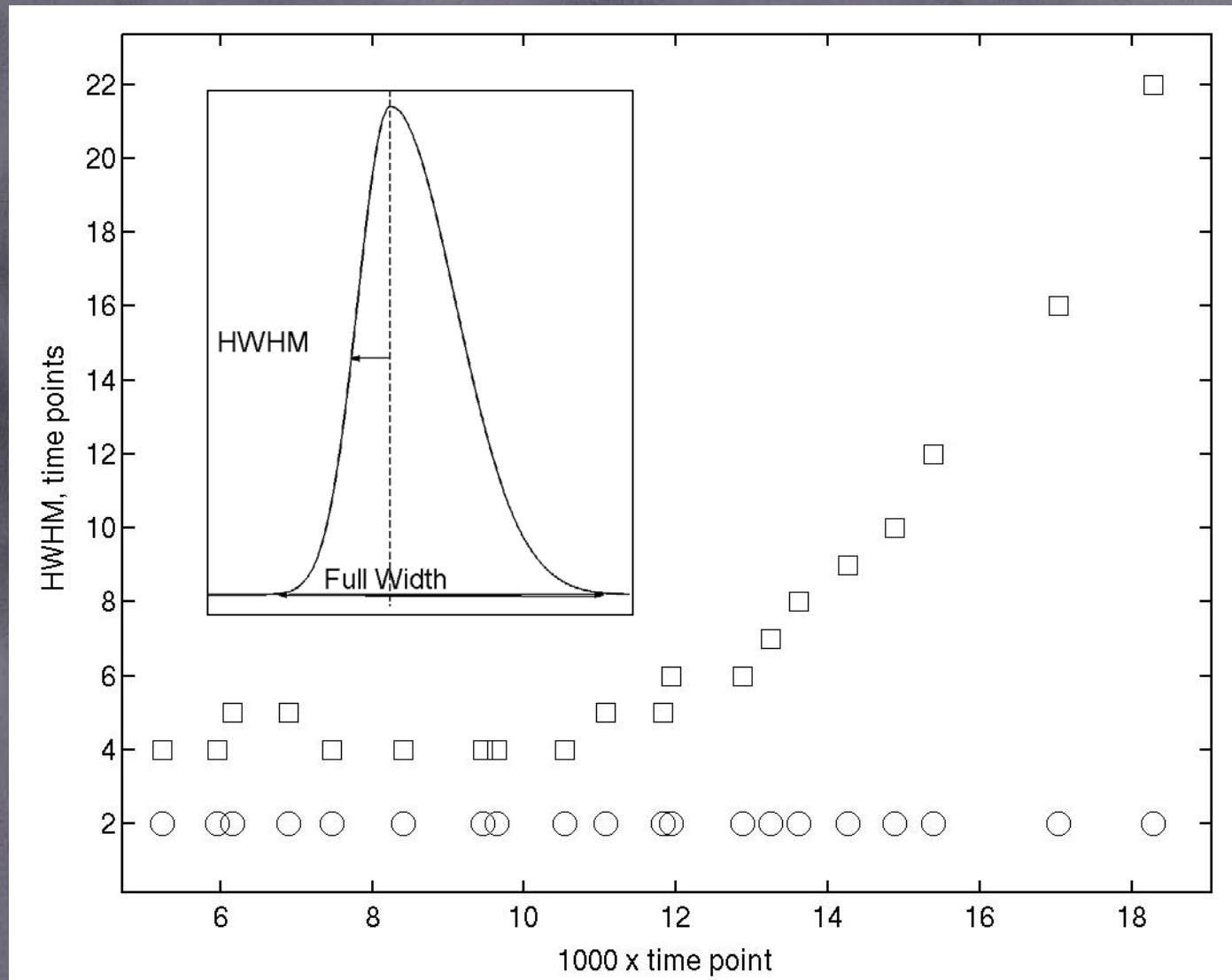
Peak location, intensity, relevance



➤ Subposition de-jittering during acquisition

SELDI Resolution in Time

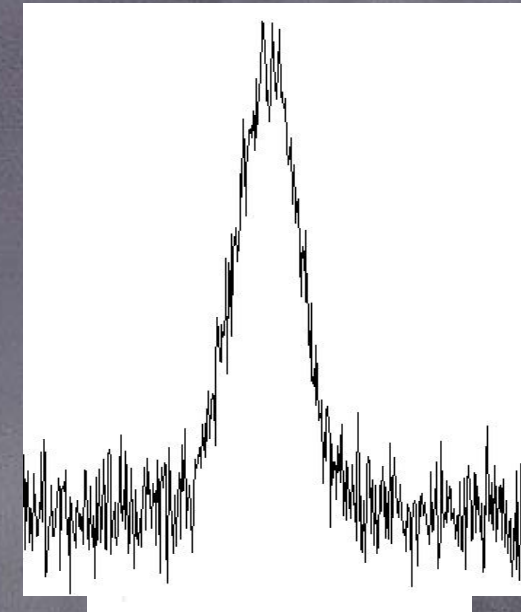
Peak size and location



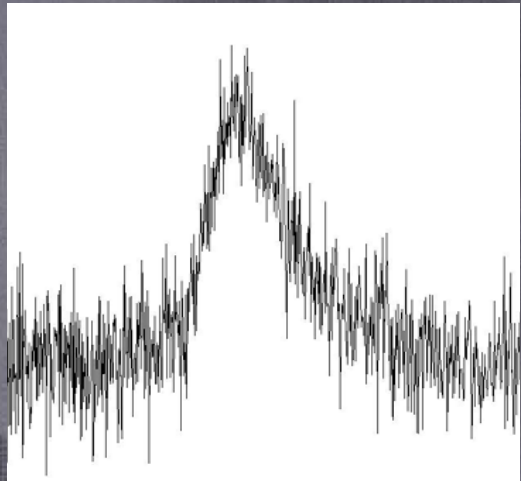
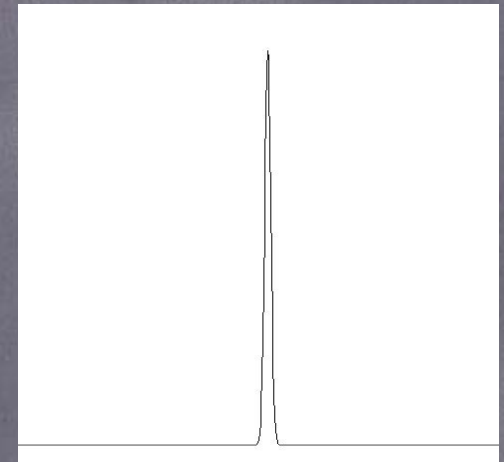
➤ $\sigma_t = \text{const} (< 12 \text{ kDa})$: monoisotopic target (Na) can be used in time

Shaping and Spiking Target Filter

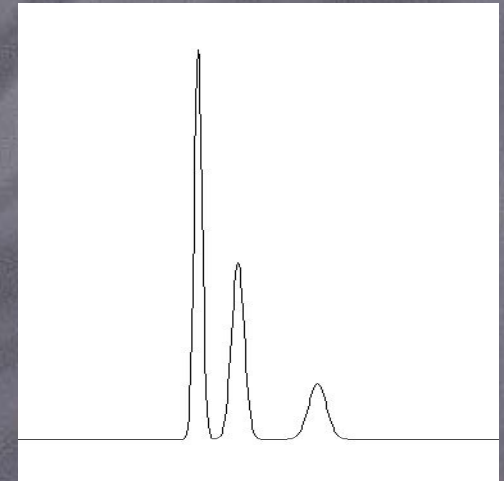
Peak location, intensity



shaping
 W_1^-
denoising

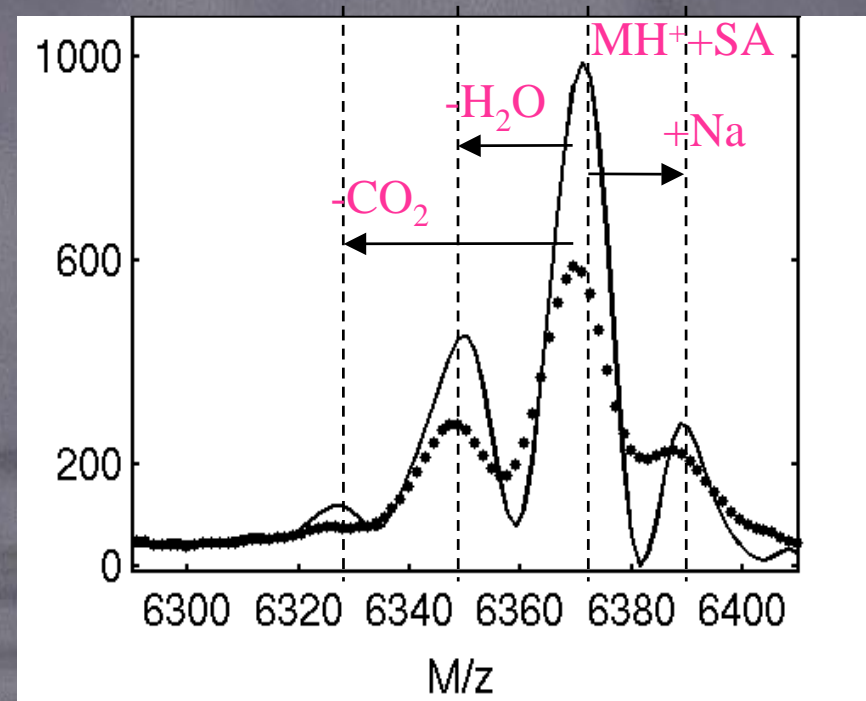
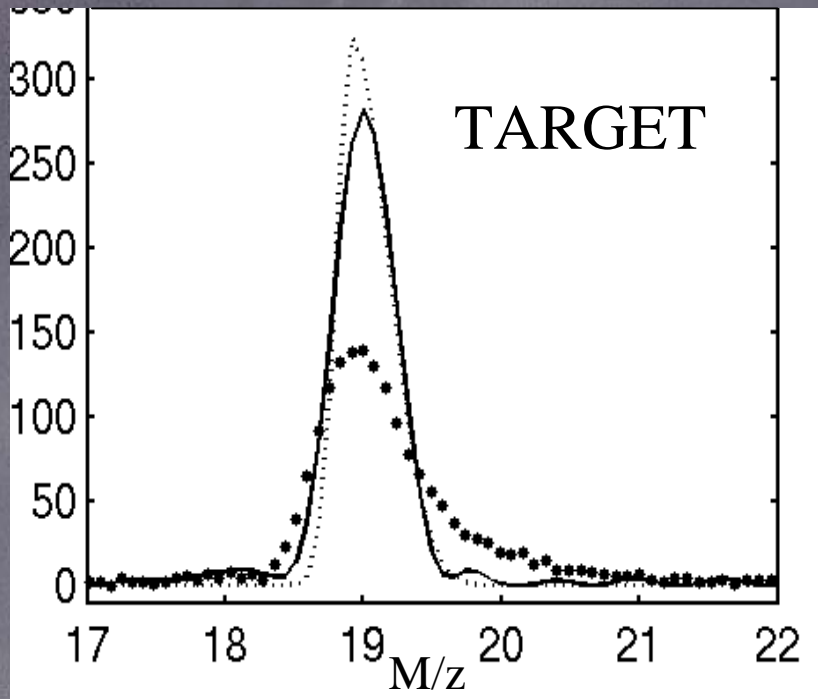


W
deconvolution



Deconvolution of SELDI TOF

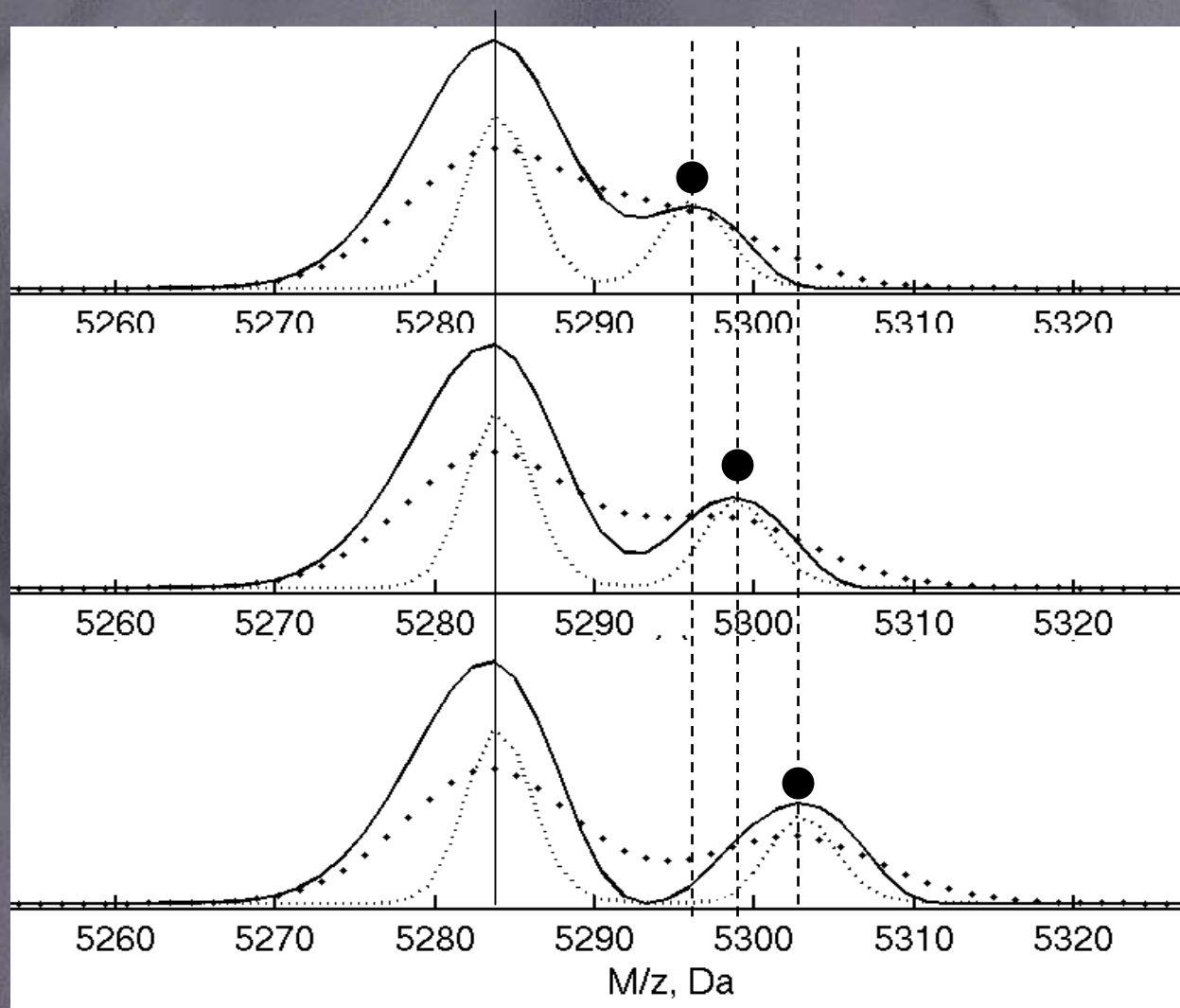
Peak location, intensity, relevance



- Na & SA adducts and H₂O, NH₄ & CO₂ (neutral loss) peaks are detected up to 9 kDa
- Adduct peaks are correlated

Spiking Accuracy

Peak location and size



- Target filter preserves total intensity
- Experimental filter detects peak shifts $< \sigma_t$ in simulated data

Conclusions:

- Noise characterization and reduction:
 - baseline removal
 - detector saturation correction
 - SNR rescaling
- Location calibration:
 - correlative dejittering
- Resolution enhancement;
 - target filter deconvolution

Acknowledgements



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