

Hands-on: Spectral Data Analysis

Python/R for Spectral Analysis

- Libraries: NumPy, SciPy, Matplotlib, pandas
- Baseline correction: Polynomial, asymmetric least squares
- Peak fitting: Gaussian, Lorentzian, Voigt
- Multivariate: PCA, PLS-DA for classification
- Quality metrics: SNR, resolution, reproducibility

```
import scipy.signal as signal
peaks, _ = signal.find_peaks(spectrum, height=0.1)
```