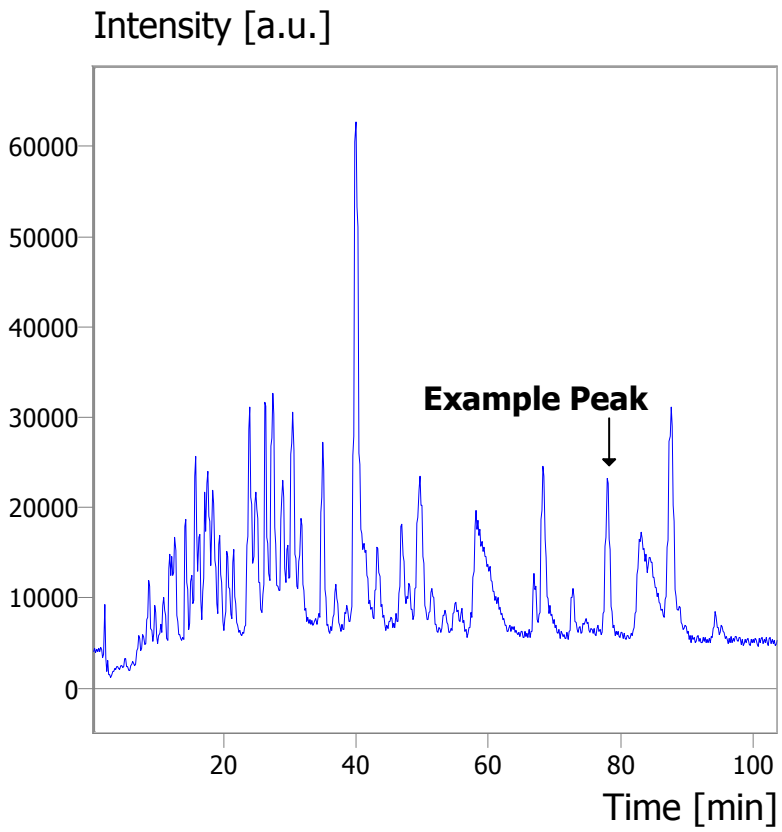
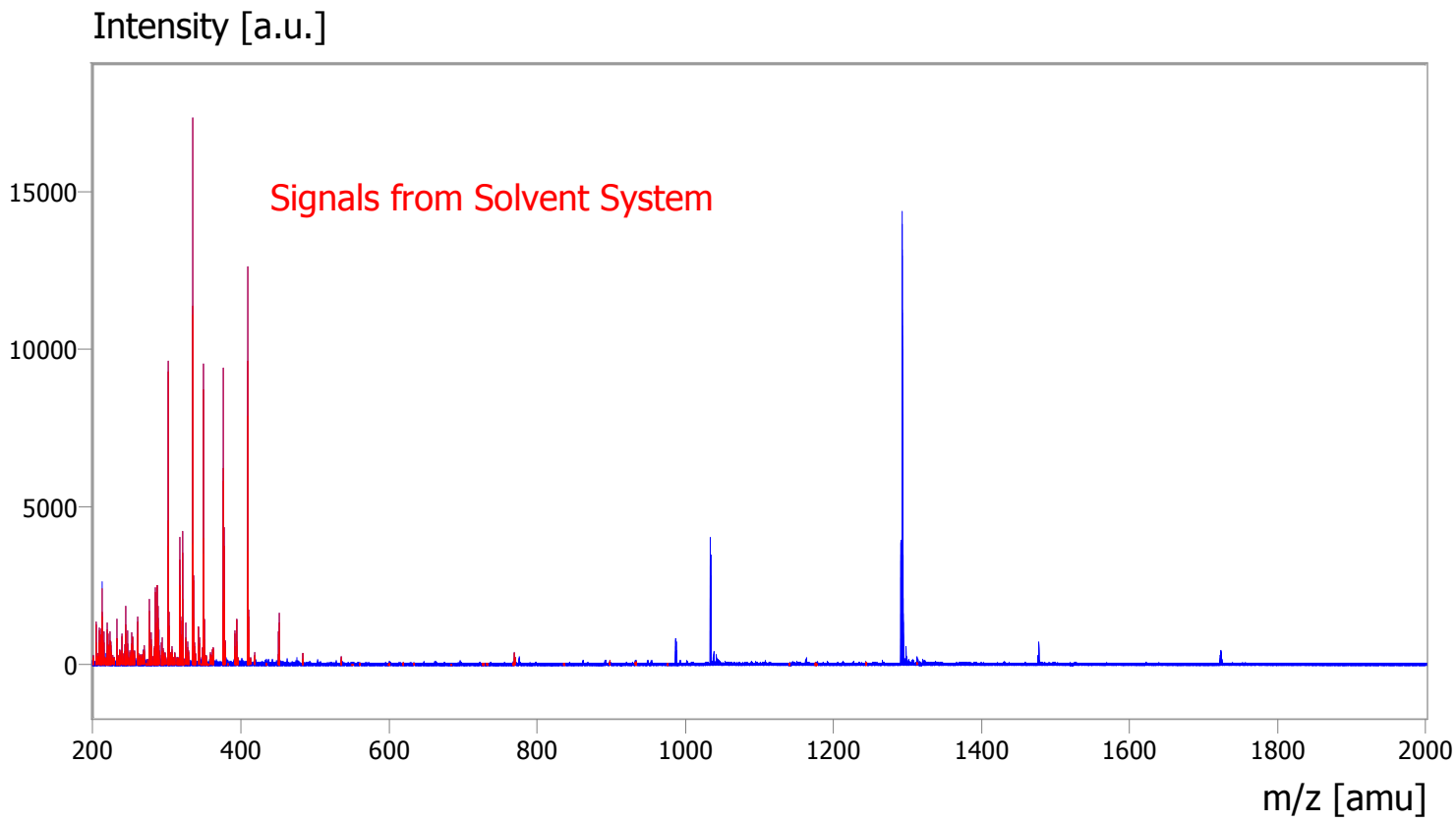
Background Removal - TIC Chromatogram of Example Data Set



Characteristics of Example Data Set

- Tryptic map of IgG1 mAb
- ESI-Tof, resolution 8000 (FWHM)
- LC Solvent: ACN/H_2O/TFA plus TFA-Fix

Background Removal – Mass Spectrum of Example Peak



Background Removal – Type 1 Signals

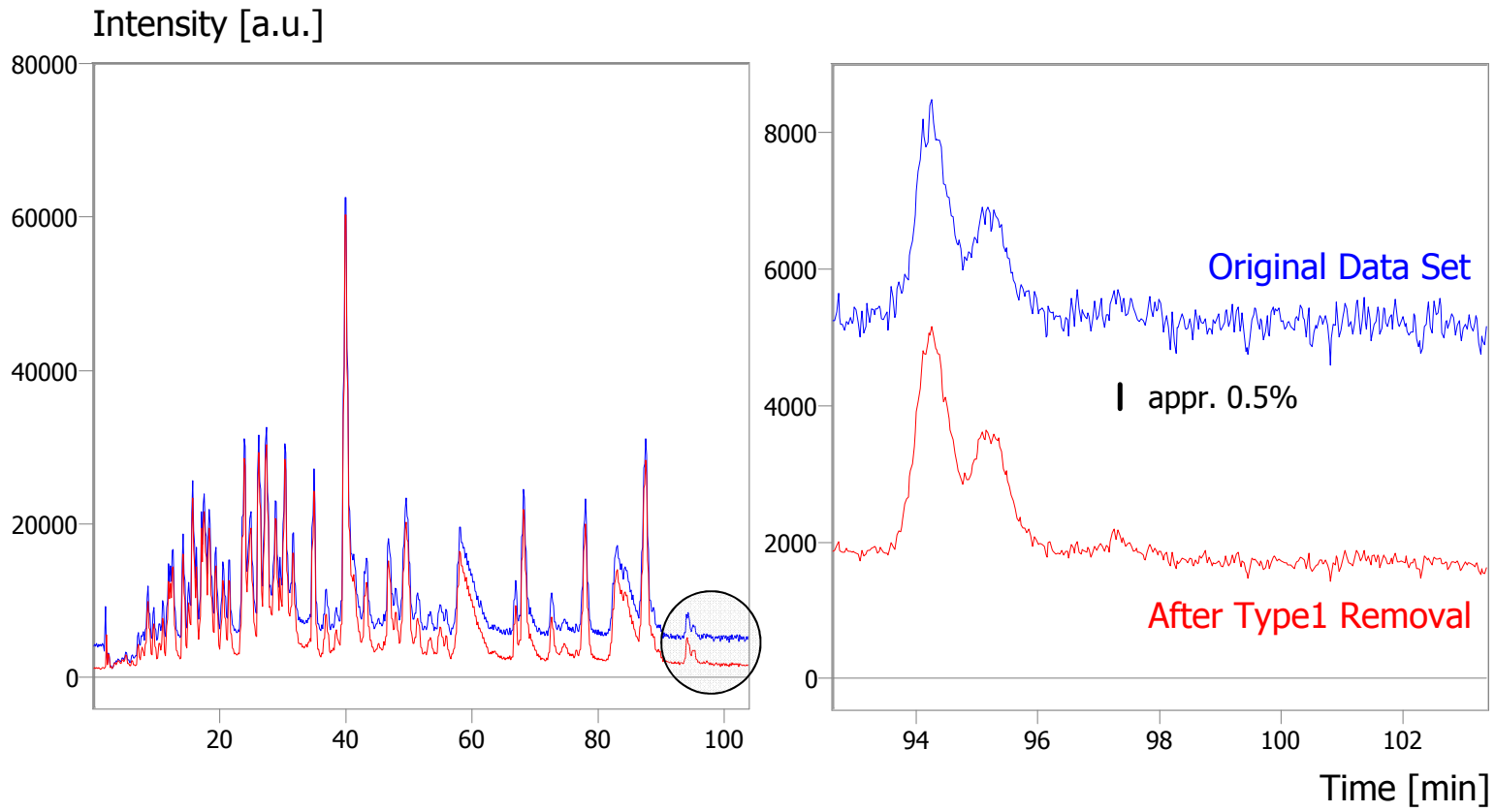
Nomenclature

- Signals from solvent system or ionization gases $\leftrightarrow$ Type1 signals

Type1 Removal by *MassMap*

- m/z Values of type1 signals $\leftrightarrow$ m/z values observed in sufficient number of consecutive scans
- Testing of ion current chromatograms for all type1 m/z values
  $\rightarrow$ Features corresponding to chromatographic peaks not removed

Background Removal –TIC Chromatograms of Example Data Set



Background Removal – Type 2 Signals

Nomenclature

- Nonspecific low-intensity signals $\leftrightarrow$ Type2 signals

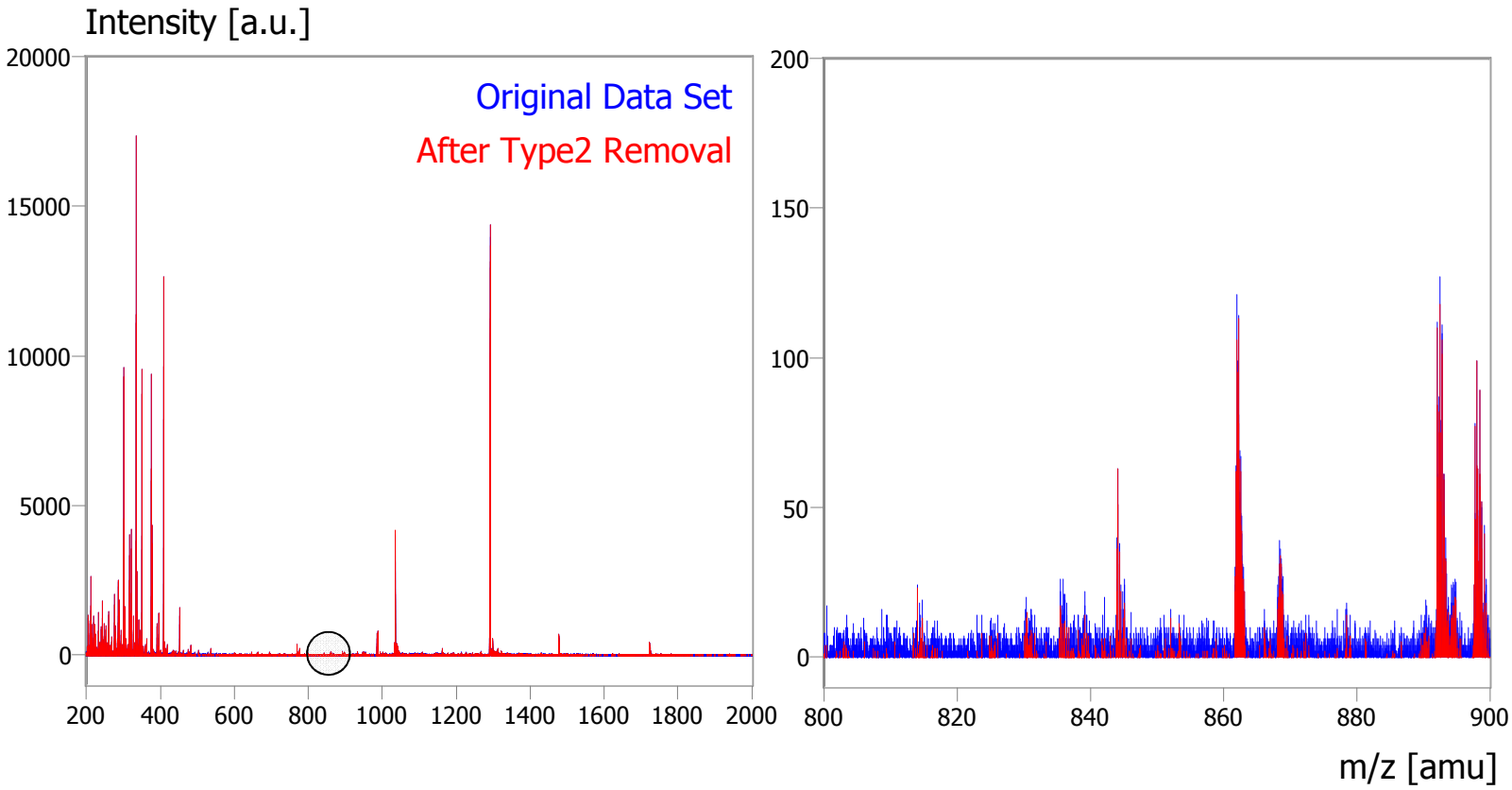
Motivation for Removal of Low Intensity Noise

- Less memory needed for backup and storage
- Significantly less computing power needed for evaluation

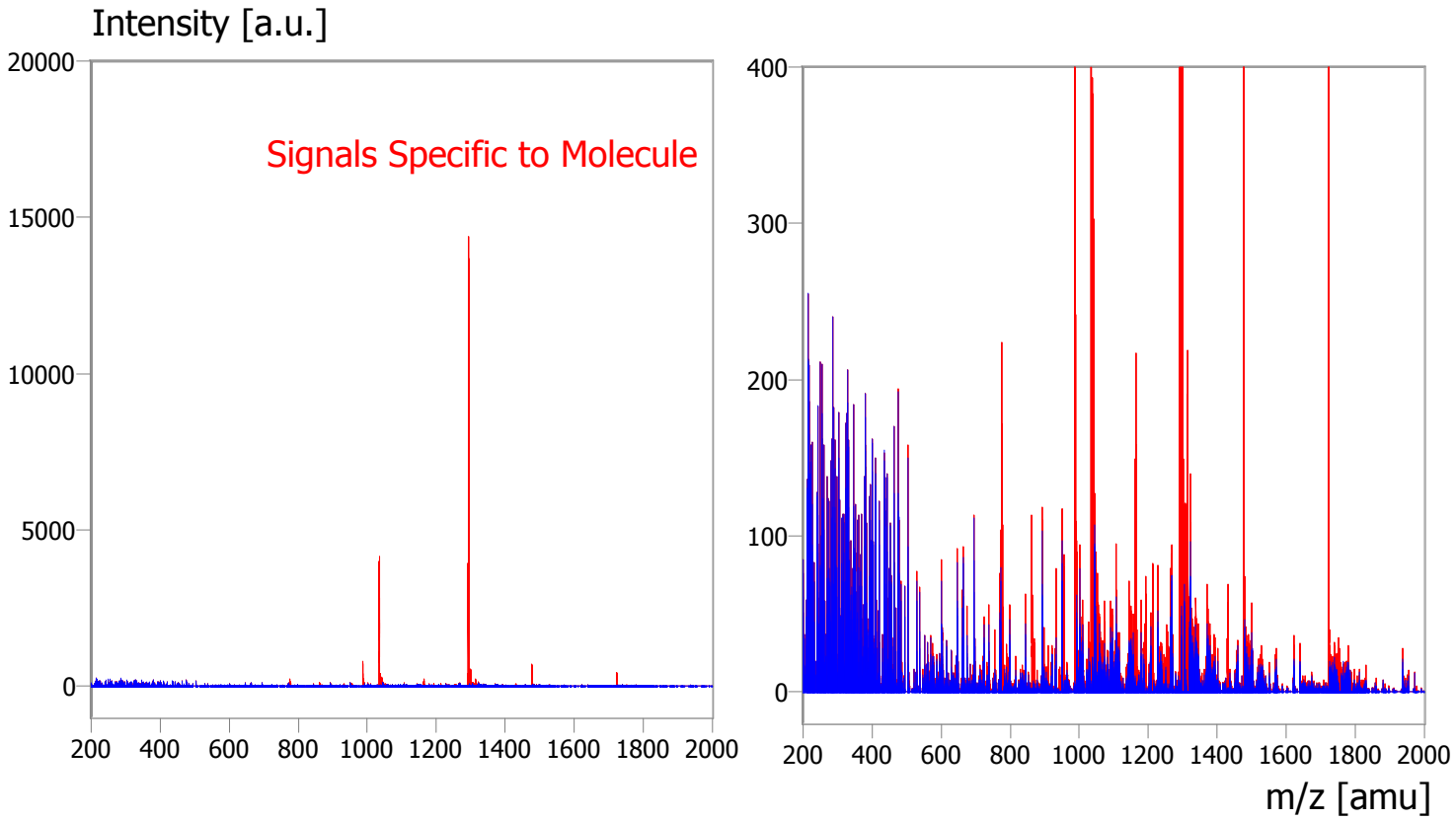
Removal of Type2 Signals by *MassMap*

- Reduction of file sizes by a factor of approximately 3
- Algorithm implemented does not lead to loss of relevant signals.

Background Removal – Mass Spectra of Example Peak



Background Removal – Residual Signals of Example Peak



Background Removal – BIC Chromatograms

Nomenclature

- **B**ackground corrected total **I**on **C**urrent chromatograms

  ↕

  Total ion current chromatograms w/o consideration of low intensity residual signals

Characteristics of Signals not Considered and of BIC chromatograms

- Intensity of residual signals dependent on intensity of main signals and eluent composition
  → Cutoff values determined by statistical analysis of individual scans
- Significant increase of sensitivity of detection in case of non-targeted analyses
  → Molecules with relative abundance down to 0.01% detectable (*Needle in a Haystack*)