

## NIST Mass Spectral Data, Tools & Documentation

**Coming in June!** - Release of our 2026 Mass Spectral Libraries

[Electron Ionization \(EI\)](#) ↗, [Tandem \(MS/MS\)](#) ↗

Visit our Booth (720) or Monday Breakfast (7 am, Room 7AB Convention Center) at the ASMS Meeting in San Diego

### GC/MS (EI & RI)

[NIST Overview](#) ↗

[EI Search Program \(Demo\)](#)

[GC Retention Indices](#)

[Free EI Libraries](#)

### LC-MS/MS (Tandem)

[NIST Overview](#) ↗

[Tandem Search Program \(Demo\)](#)

[Peptides](#)

[Free Tandem Libraries/Utilities](#)

### MS Tools

[MS Interpreter](#)

[AMDIS \(GC/MS\)](#)

[MS Pepsearch](#)

[Library Builder \(Lib2NIST\)](#)

### Other Information

[Papers/Presentations](#)

[Distributors](#)

[NIST Chemistry Webbook](#) ↗

[Dart Forensics](#)

## Our New Website

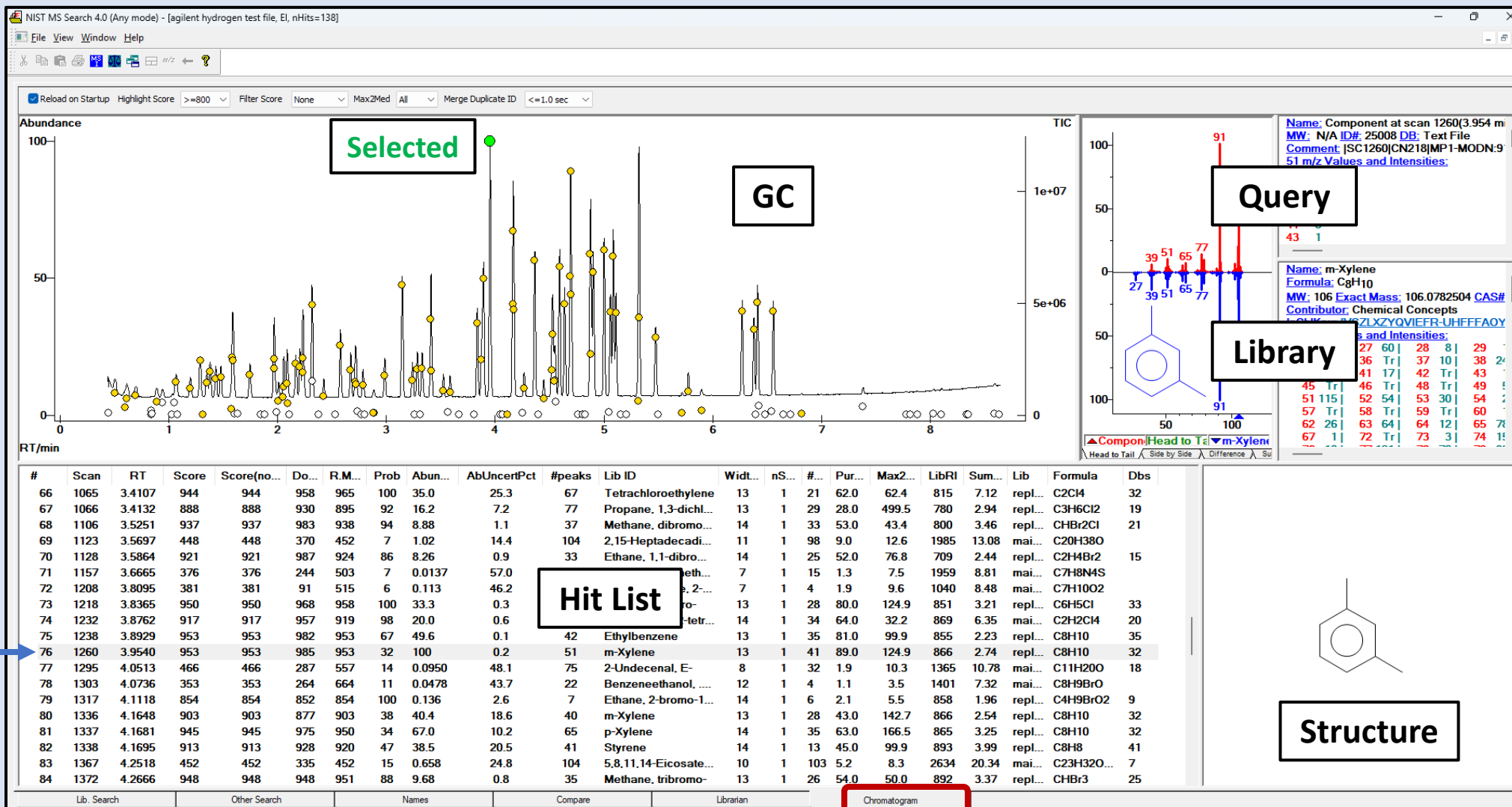
- Information
- Software
- Free data

[Chemdata.nist.gov](https://chemdata.nist.gov)



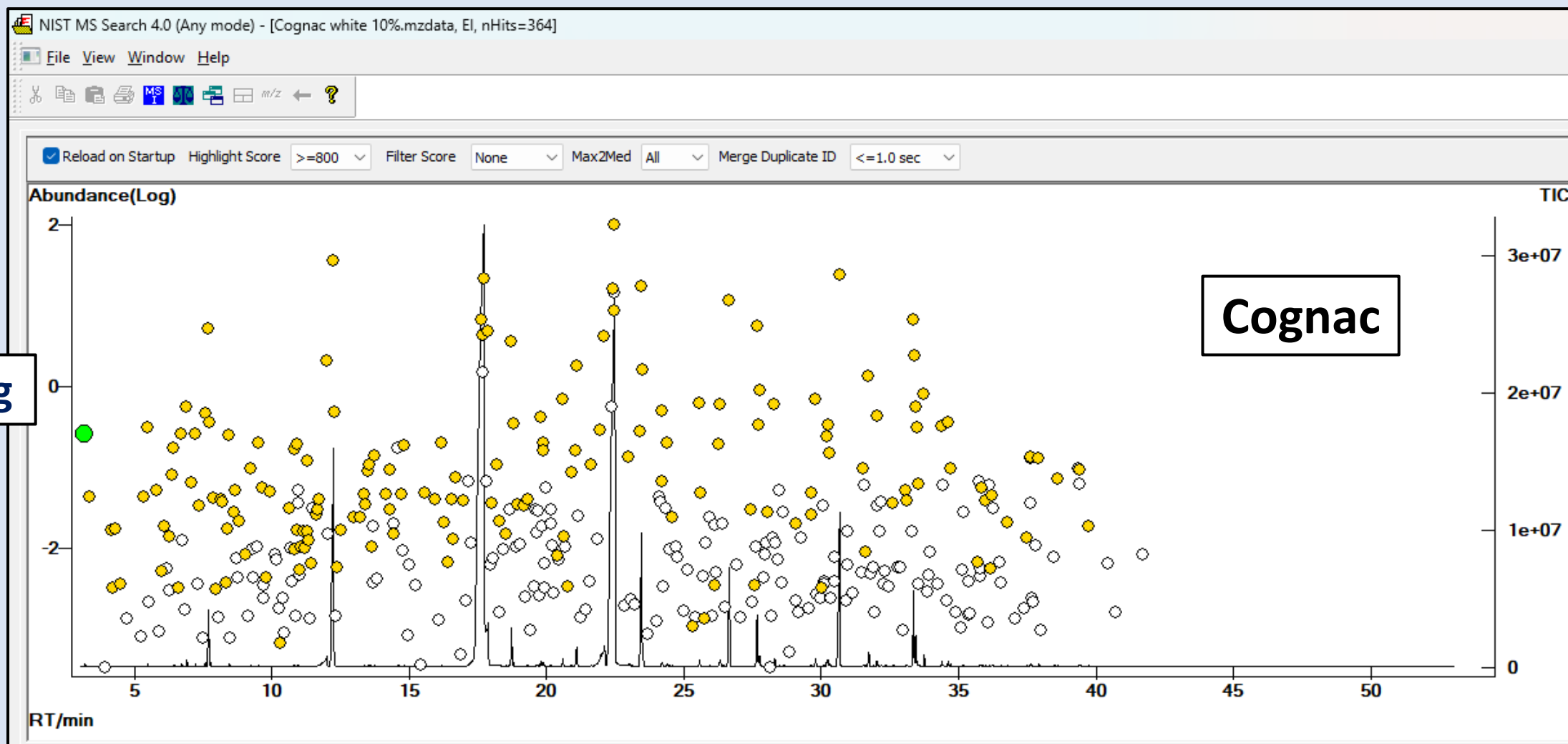
NIST26

# GC/MS AMDIS Analysis

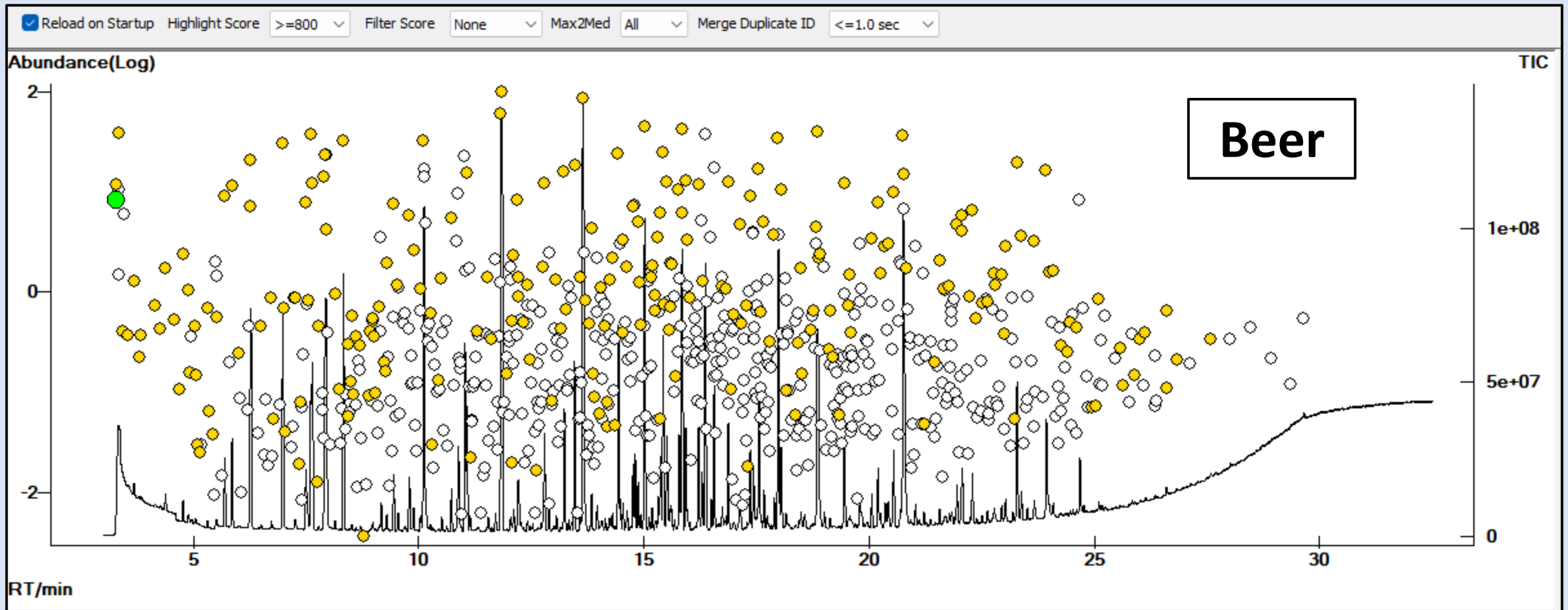


Standard mix

# Low Resolution EI with AMDIS

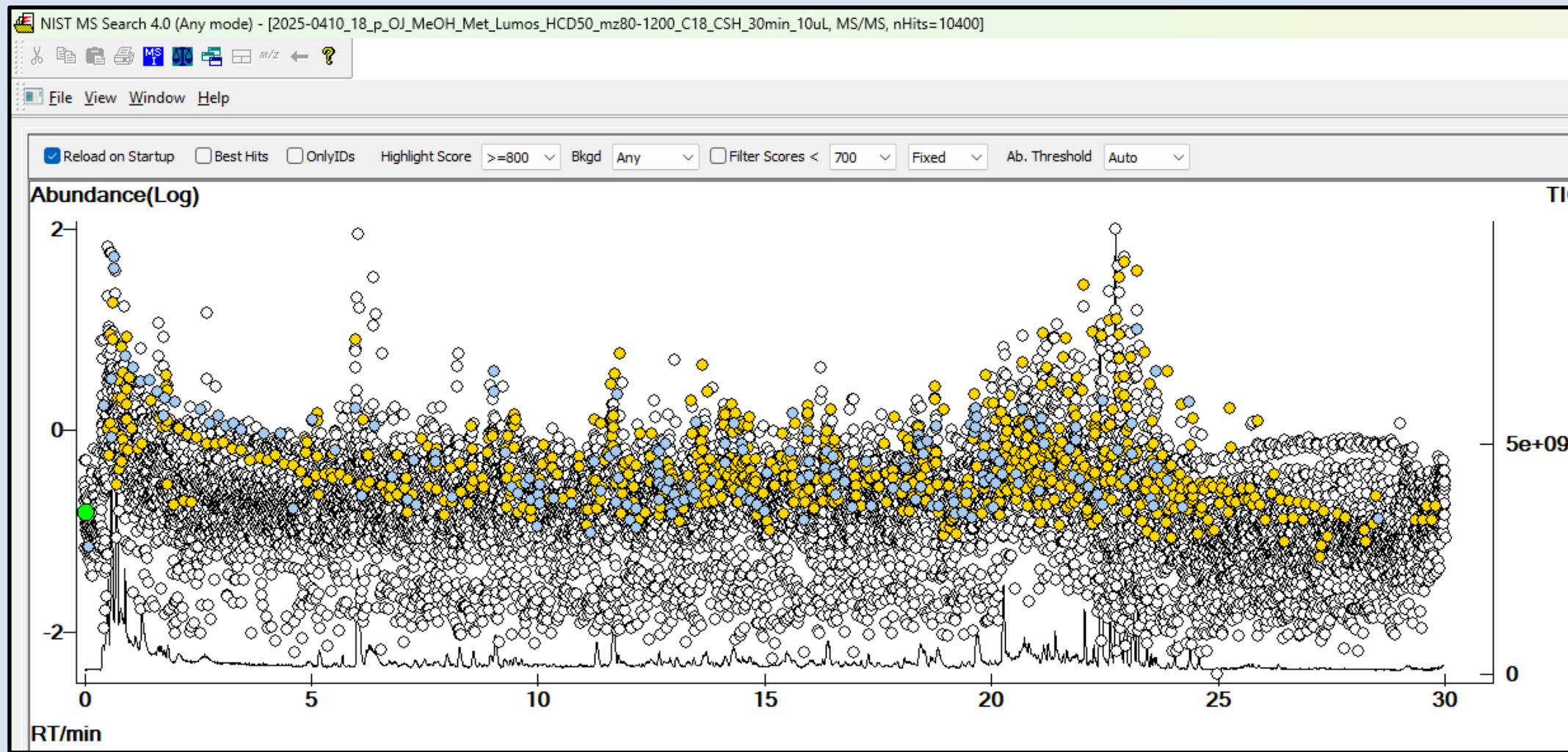


# High Resolution EI with AMDIS



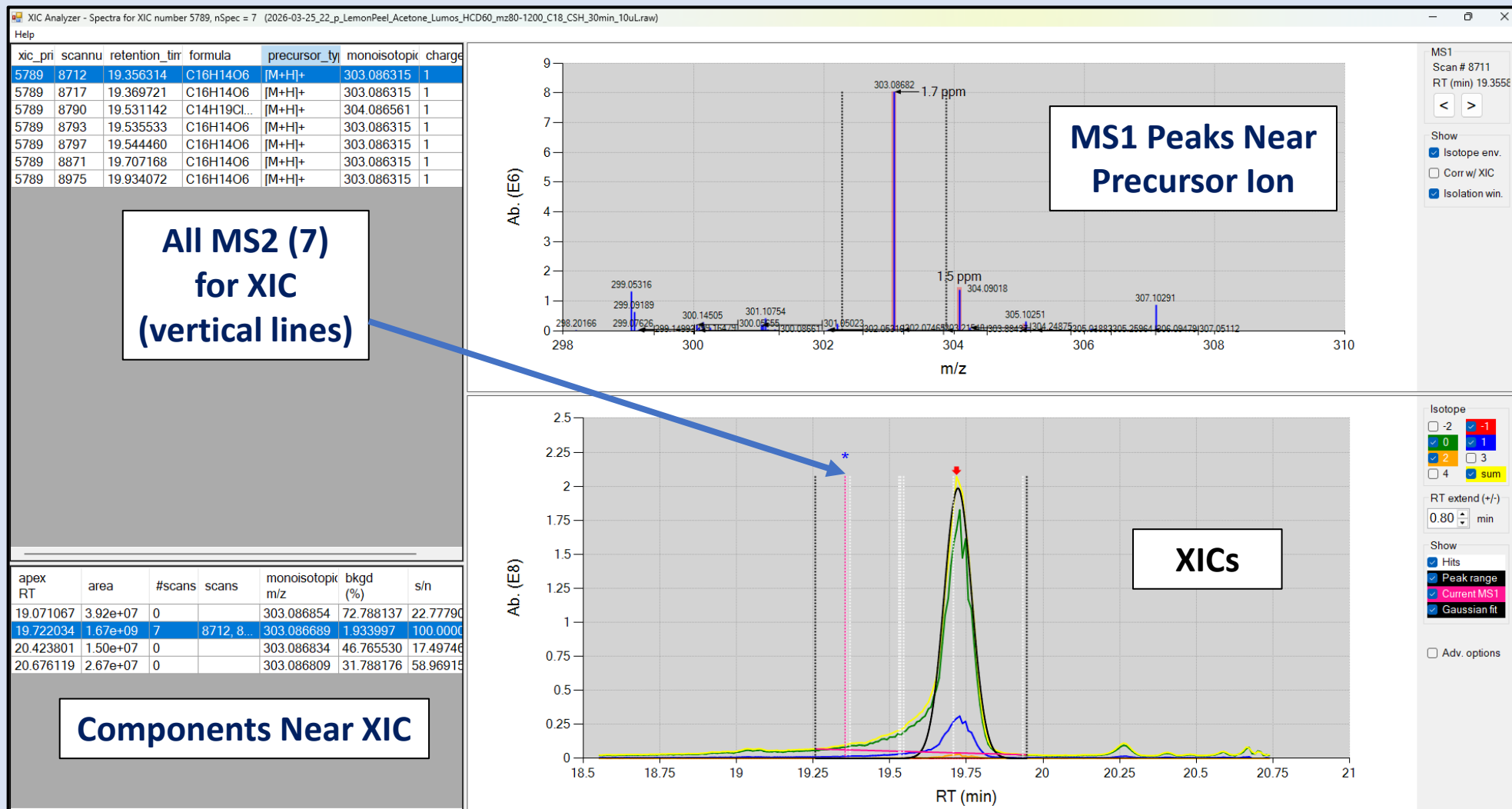
High resolution improves spectrum deconvolution

# LC/MS2 – Orange Juice



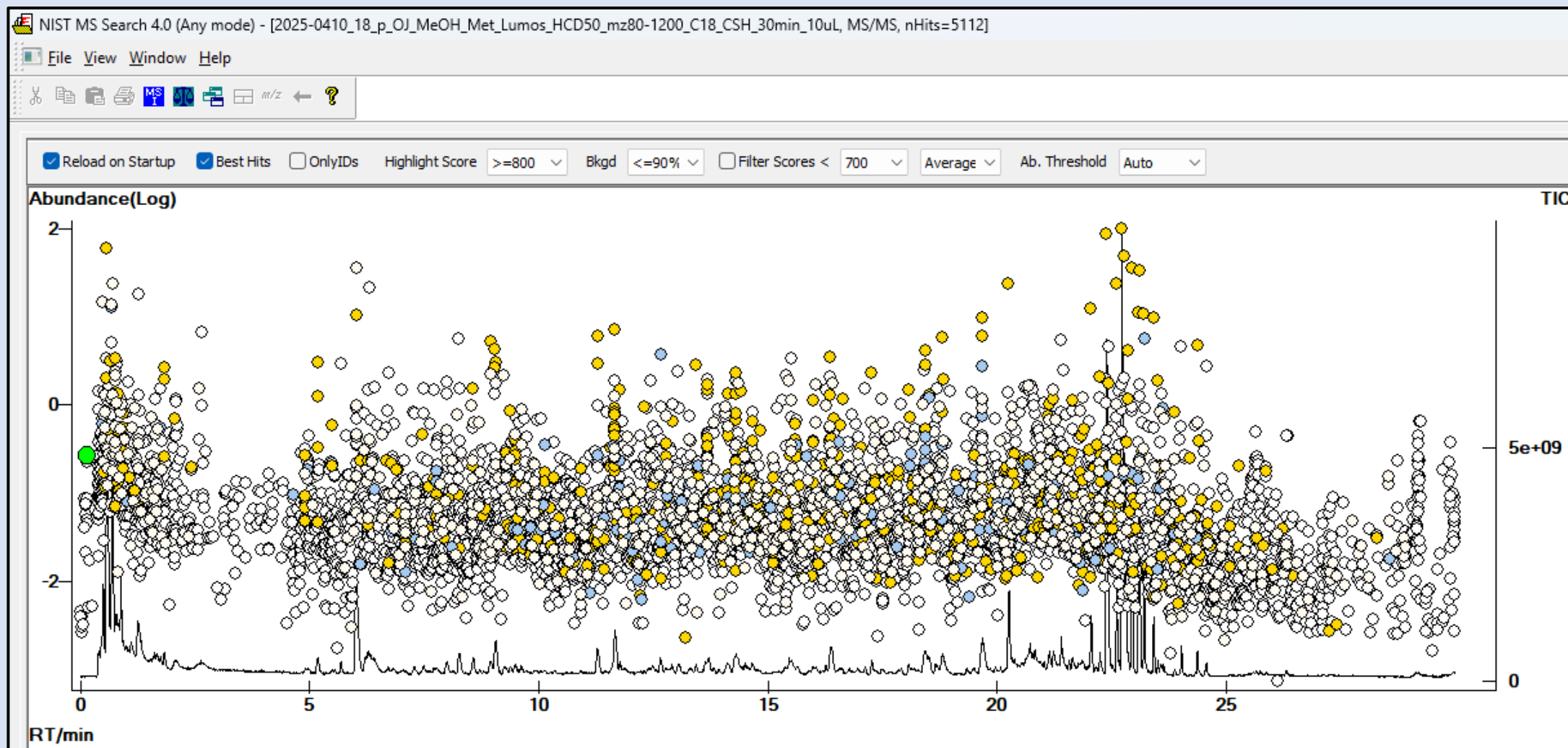
● ID ● In-Source

# XIC Analyzer – Connect MS2 Spectra to MS1



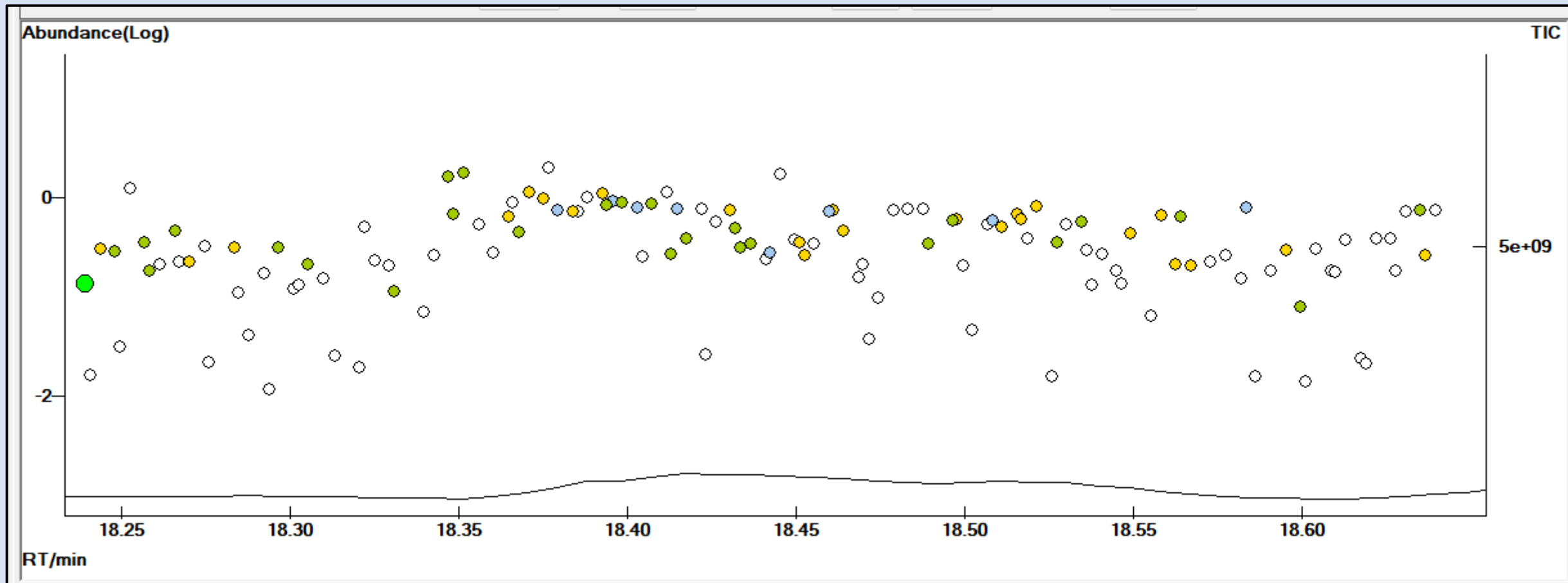
G.Wang et al. "An XIC-Centric Strategy for Improved Identification and Quantification in Proteomic Data Analyses" Journal of Proteome Research (2024)

# Orange Juice - LC/MS-MS - XIC + Filter



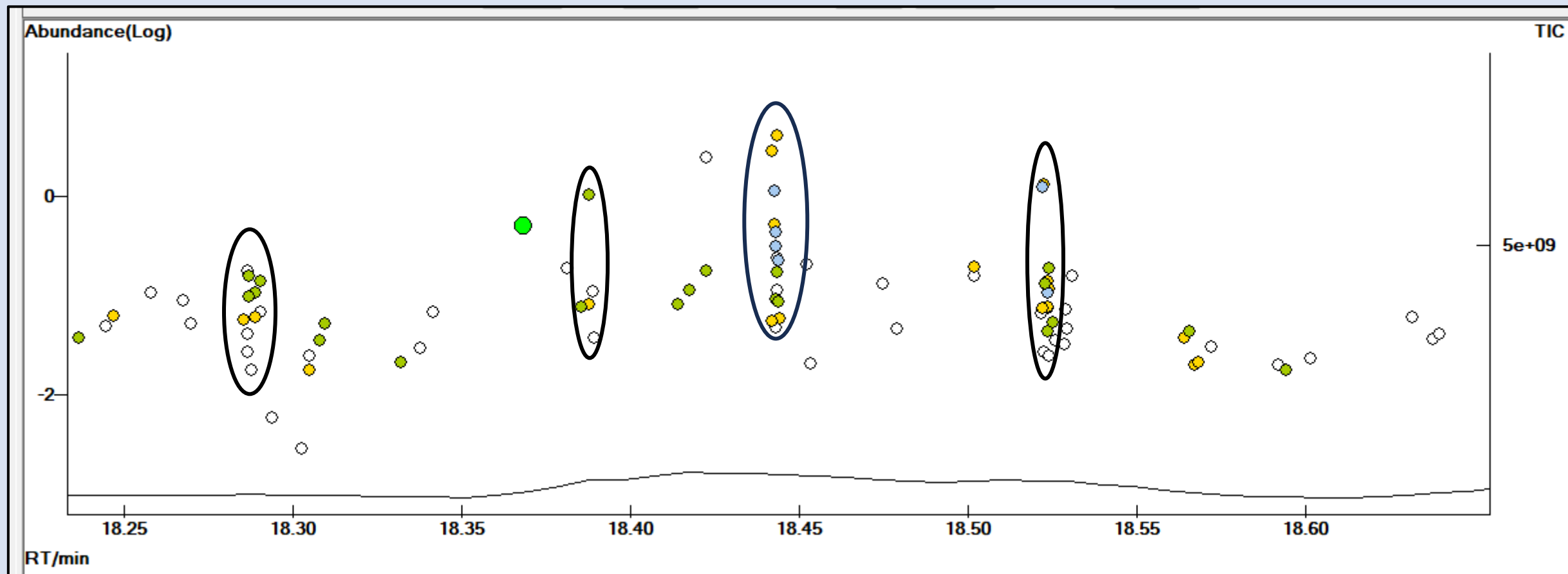
● ID ● In-Source

# MS/MS Spectra: 30 sec Interval

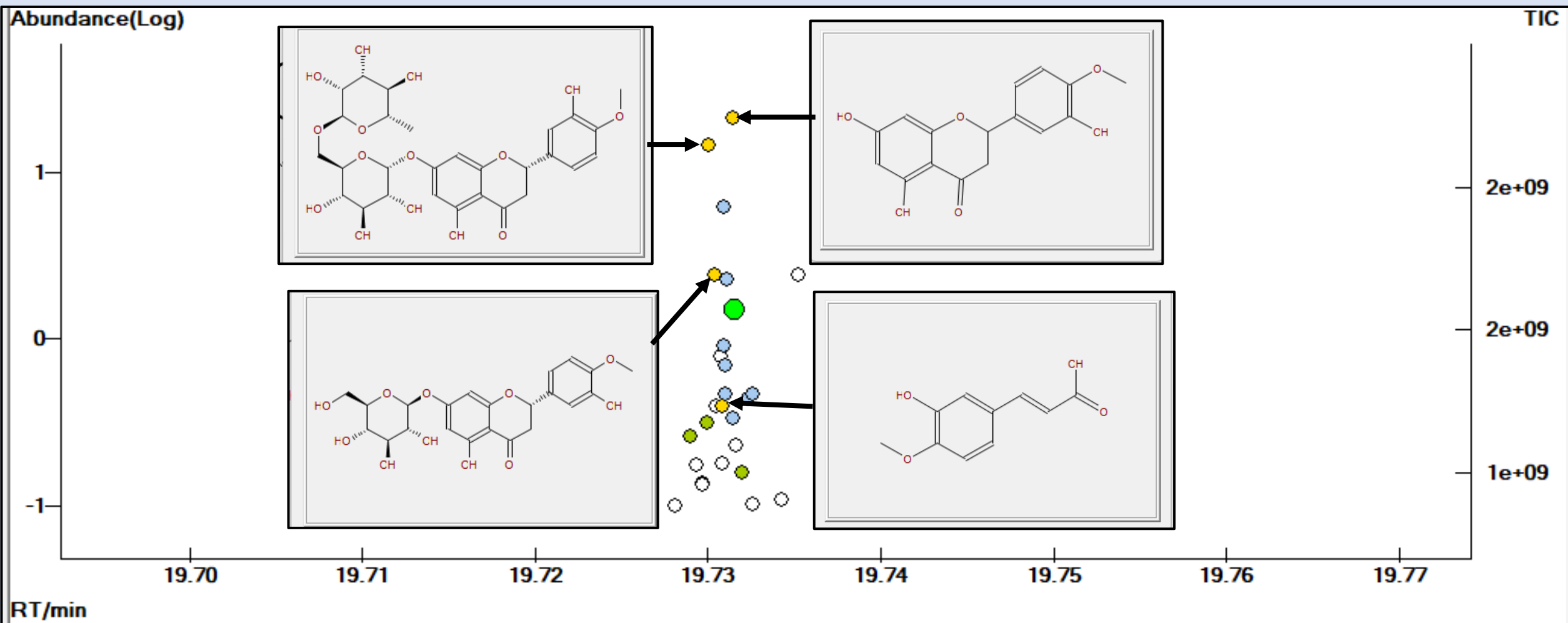


○ ID    ● In-Source    ● Hybrid

# After XIC Analysis



# Orange Juice



Width ~ 0.2 sec.