

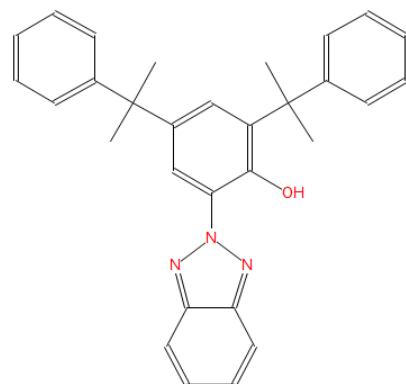
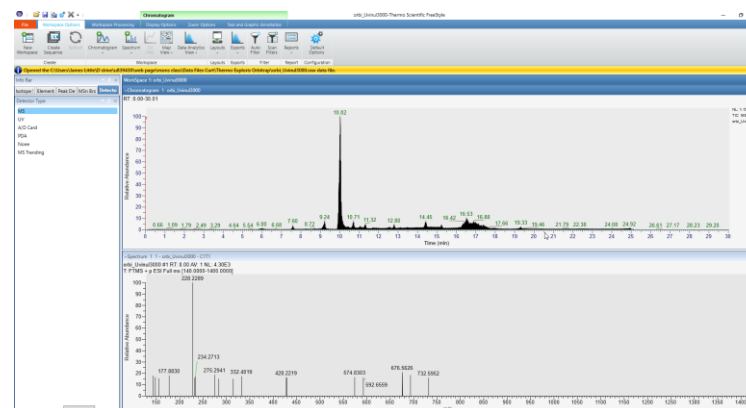
Elemental Composition with Freestyle

Mass Spec Interpretation Services

11/06/2025

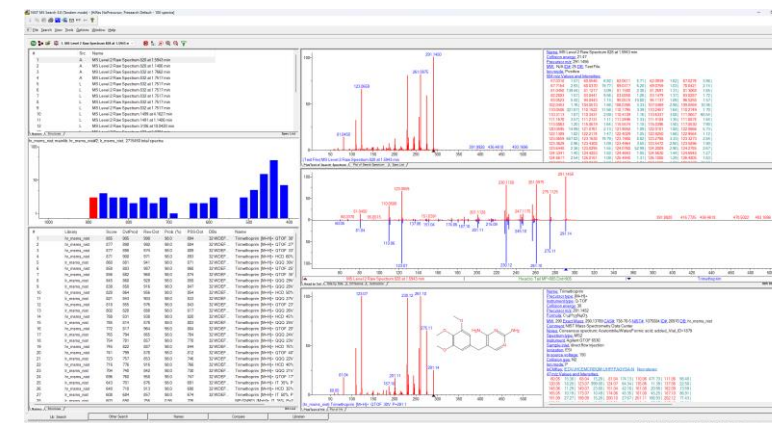
NIST MSMS Search

The diagram illustrates a hybrid experimental setup for studying ion-atom interactions. An **ion packet** is trapped in a **C-trap** (Paul trap). Simultaneously, an **atom** is trapped in an **Orbitrap analyzer**. The atom's axial motion is detected by a **Voltage ramp**, which produces a **Detected signal** (represented by a sine wave). The detected signal is then processed by an **Amplifier**.



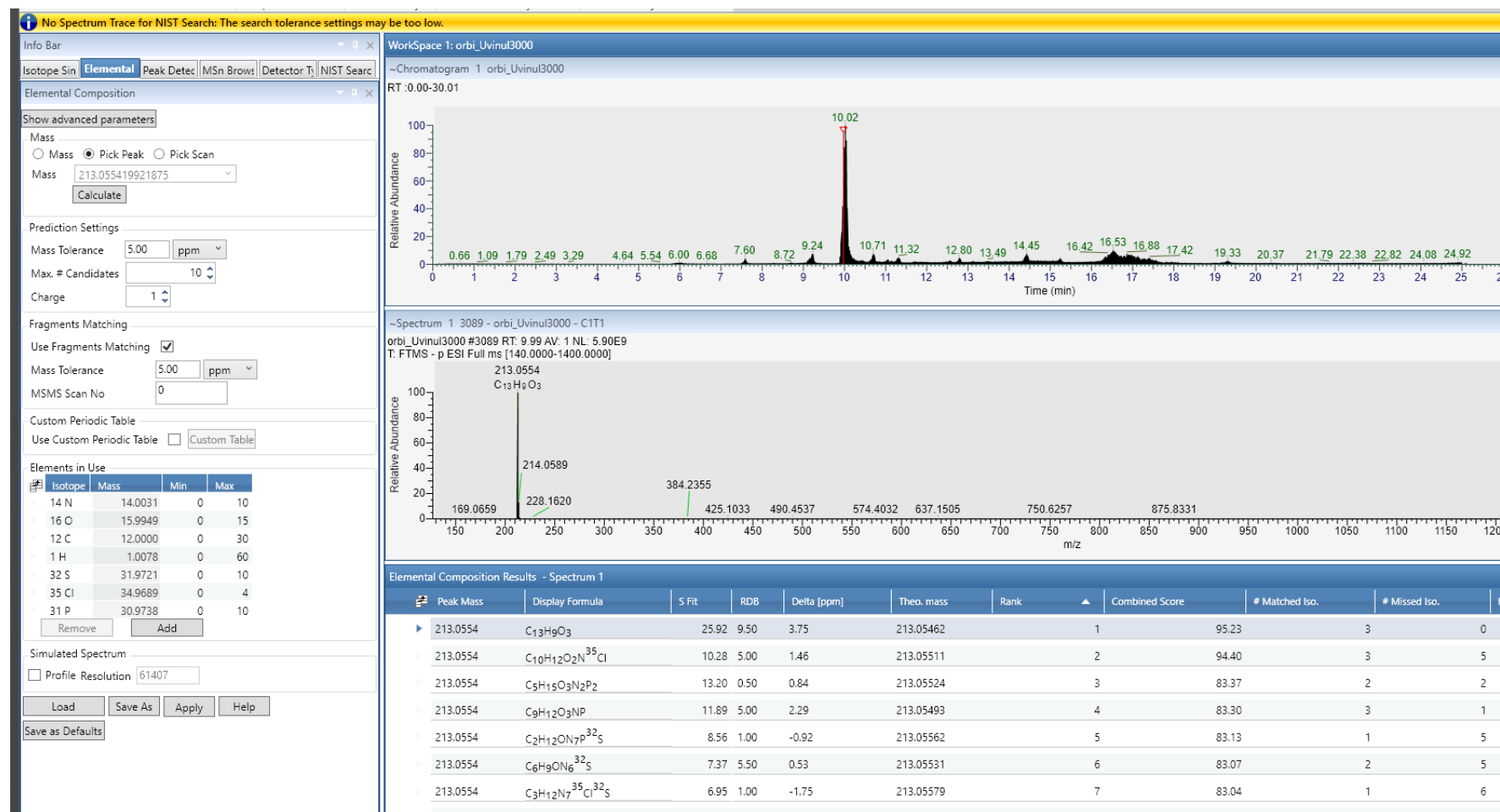
Formula: C₃₀H₂₉N₃O

MW: 447 Exact Mass: 447.231062 CAS#: 70321-86-7 |



- *Excellent Accurate m/z Measurements for Molecular Formula Determinations*
- *Excellent Isotope Ratios*
- *Utilizing **Both Minimizes** the Number in Results List*

- Open the Elemental Tab
- Setup whichever elements and element ranges are appropriate
- Click on Pick Peak mode
- Click on an ion mass value in an MS1 Spectrum window
- Value should be automatically transfer to Elemental window in “mass” box
- Click on calculate
- Values will be displayed in a window that opens below spectrum window
- Can do for an average spectrum **or** single spectrum



Chromatogram

File Workspace Options Workspace Processing Display Options

Detect Peaks Add/Delete Peak Peaks List Manual Noise Range Import Component

Peak Detection Component Detection

No Spectrum Trace for NIST Search: The search tolerance settings may be too low.

Info Bar: Isotope Sin **Elemental** Peak Detect MSn Brows Detector T₁ NIST Search

Elemental Composition

Show advanced parameters

Mass
☐ Mass ☒ Pick Peak ☐ Pick Scan
 Mass: 213.055419921875
 Calculate

Prediction Settings
 Mass Tolerance: 5.00 ppm
 Max. # Candidates: 10
 Charge: 1

Fragments Matching
 Use Fragments Matching: ☒
 Mass Tolerance: 5.00 ppm
 MSMS Scan No: 0

Custom Periodic Table
 Use Custom Periodic Table: ☐ Custom Table

Elements in Use

Isotope	Mass	Min	Max
14 N	14.0031	0	10
16 O	15.9949	0	15
12 C	12.0000	0	30
1 H	1.0078	0	60
32 S	31.9721	0	10
35 Cl	34.9689	0	4
31 P	30.9738	0	10

Remove Add

Simulated Spectrum
☐ Profile Resolution: 61407
 Load Save As Apply Help
 Save as Defaults