AutoRIX and Beyond: Empowering GC/ID 5.1 for Enhanced Compound Identification

New GC/ID version 5.1 Suite

The release of GC/ID version 5.1 introduces a suite of powerful features designed to elevate the accuracy, efficiency, and user experience of GC/MS analysis. At the forefront of these advancements is AutoRIX, a revolutionary technology that redefines Retention Index (RI) calibration.

AutoRIX: The Intelligent RI Calibration Solution

The accuracy of compound identification in GC/MS hinges on not only library search, but precise RI calibration. However, achieving a clean RI calibration, free from interfering peaks, can be a persistent challenge. AutoRIX tackles this challenge head-on, employing a sophisticated blend of library searching and a patented algorithm to accurately identify and assign RI standard peaks, even in the face of impurities, background bleed, or solvent masking.

AutoRIX in Detail

AutoRIX's patented algorithm combines the power of search with a patented algorithm for predicting the retention times and intensities for heavier n-alkanes, which normally are difficult to correctly identify. This enables the automatic assignment of the correct carbon numbers to peaks in the RI standard, even in the presence of column bleed, interferences, or poor signal-to-noise ratios.

AutoRIX N-Alkane Standards

Furthermore, AutoRIX intelligently handles scenarios where n-alkane standards lack consecutive carbon numbers. While this is not generally recommended, AutoRIX can still accurately identify RI standard peaks, showcasing its adaptability to diverse calibration standards (Figure 1).
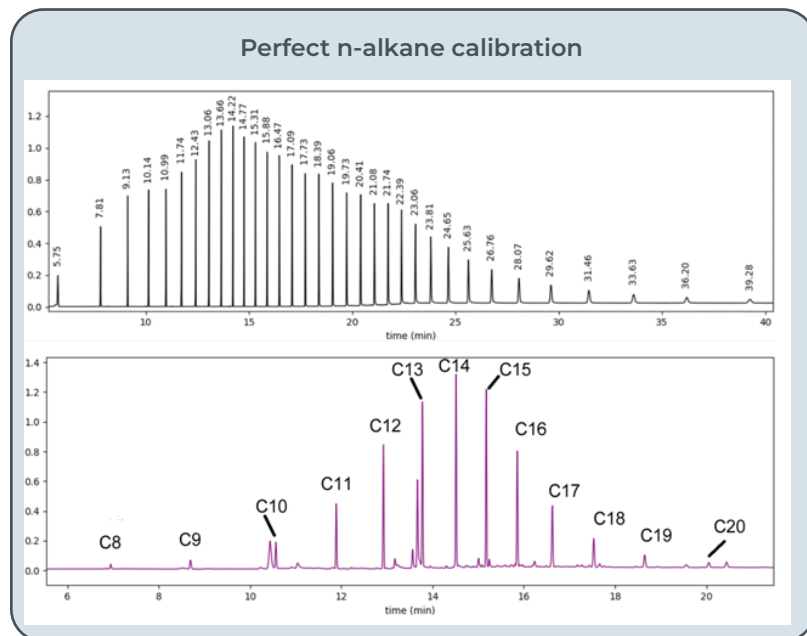

Figure 1. AutoRIX n-alkane calibration. The top plot is a perfect n-alkane calibration with no impurity peaks from C9-C40. The bottom plot contains significant impurity peaks many which are bigger than some of the C? standards. AutoRIX will try and automatically find and identify the RI standard peaks.

Key Features and Benefits of AutoRIX

- **Unmatched Accuracy and Reliability:** AutoRIX significantly enhances the accuracy and reliability of RI calibrations, even in challenging scenarios with impurities, background interference, or strong solvent interference.

- **Time and Cost Efficiency:** AutoRIX saves valuable time and resources by eliminating the need for pristine calibrations and reducing the risk of peak misidentification.

- **Boosted Confidence in Compound Identification:** Accurate RI calibration is fundamental for confident compound identification. AutoRIX ensures this accuracy, leading to more reliable results.

- **User-Friendly Interface:** The intuitive RI Editor allows for easy verification and editing of alkane assignments, if necessary, making AutoRIX accessible to users of all levels.

- **Handling Real-World Challenges:** AutoRIX excels in handling non-consecutive alkanes in RI standards and allows for the exclusion of solvent peaks, addressing common challenges in GC/MS analysis.

Additional GC/ID 5.1 Features

- **Enables non-n-alkane standards for RI Calibrations:** Running a validation standard that could be used for automatic RI calibration? No problem with AutoRIX.

- **Manual Peak Editing:** The new manual peak editor allows users with the ability to override automatic peak picking, adjust baselines, and modify spectral averaging regions, offering greater control over data analysis.

- **Enhanced User Interface:** GC/ID 5.1 introduces an improved user interface experience, simplifying finding and setting of key parameters.

- **Targeted Analysis:** The ability to mark and filter target compounds streamlines workflows and focuses analysis on compounds of interest.

- **User Library Expansion:** Users can now seamlessly add spectra and RI data from their runs directly to a NIST User Library, facilitating the creation of custom libraries for specialized applications.

- **Performance and Stability Improvements:** GC/ID 5.1 is a 64-bit application, resulting in faster operation (up to 70%) and enhanced stability.

Conclusion

AutoRIX, along with the other enhancements in GC/ID 5.1, represents a significant leap forward in GC/MS analysis. By addressing the challenges of RI calibration and providing a suite of user-centric features, GC/ID 5.1 empowers scientists to achieve more accurate, efficient, and confident compound identification. This translates to streamlined workflows, optimized resource utilization, and, ultimately, more impactful scientific discoveries.

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