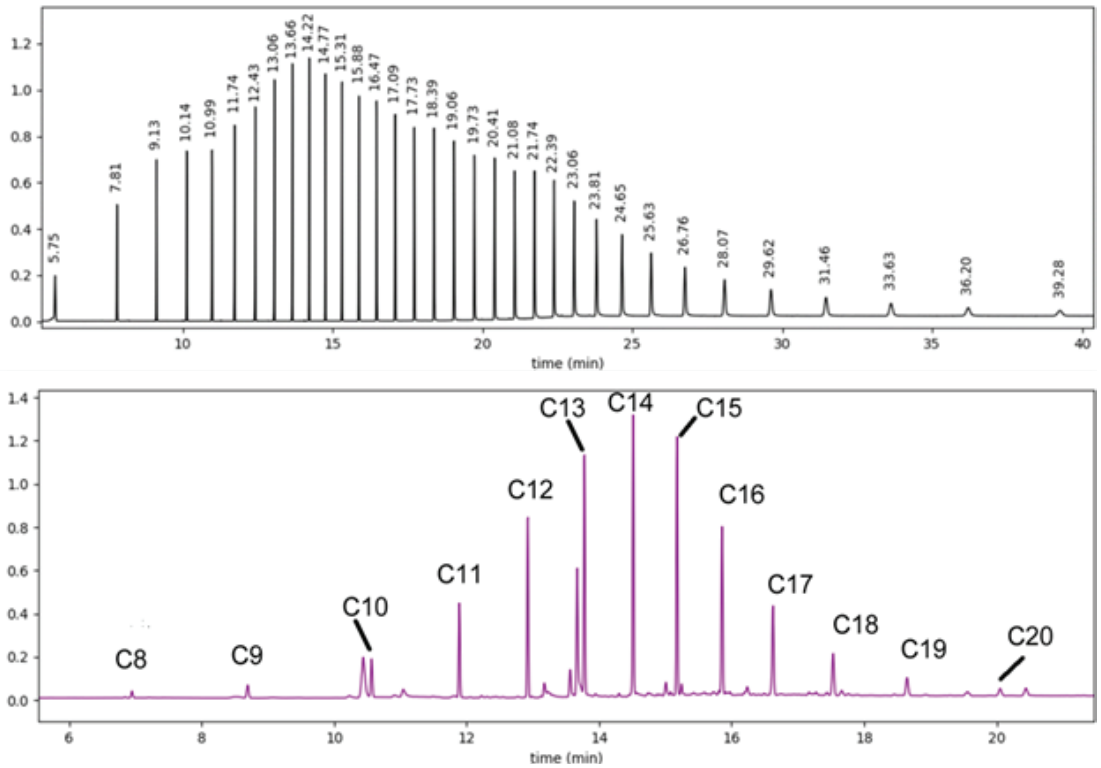
AutoRIX: Revolutionizing Retention Index Calibration in GC/MS

The Challenge of Impure Calibrations

Accurate compound identification in GC/MS relies not only on conventional library search, but also on precise Retention Index (RI) calibration. However, achieving a clean calibration run, free from interfering peaks and background interference, can be challenging. This is particularly true with sampling techniques like Solid-Phase Microextraction (SPME) or Large Volume Injection (LVI), which often introduce carryover and impurities. Traditional algorithms struggled with this, potentially misassigning standards peaks and compromising calibration accuracy. The alternative is the costly and time consuming manual peak assignments.

Introducing AutoRIX

AutoRIX, a groundbreaking feature in GC/ID release 5.1, offers a robust and intelligent solution to RI calibration challenges. It combines library searching with a patented algorithm to accurately identify and assign RI standard peaks, even in the presence of impurities or complex analytical conditions.



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.

How AutoRIX Works

- **Library Search and Peak Elimination:** AutoRIX initiates a library search on all detected peaks in the RI calibration, effectively eliminating those that are not n-alkanes.
- **Prediction of Heavier Alkanes:** For heavier n-alkane peaks, where traditional library search will falter, AutoRIX employs a predictive algorithm. This algorithm leverages elution times and relative intensities to accurately identify these challenging calibration peaks.
- **Handling Non-Consecutive Alkanes:** While not the ideal scenario, AutoRIX accommodates RI standards that lack consecutive carbon numbers, showcasing its adaptability.
- **Exclusion of Solvent Peaks:** Samples containing n-alkane solvents, like pentane or hexane, can distort RI values. AutoRIX allows for the seamless exclusion of these peaks, ensuring calibration integrity.
- **Identification of Additional Alkanes:** AutoRIX goes beyond expectations by potentially identifying additional n-alkanes present in the RI standard, even if they weren't initially specified.
- **Verification and Editing:** The RI Editor empowers users to easily verify, view, and, if necessary, edit the alkane assignments made by AutoRIX, offering control and flexibility.

Benefits of AutoRIX

- **Enhanced Accuracy and Reliability:** AutoRIX significantly improves the accuracy and reliability of RI calibrations, even in challenging scenarios with impurities or complex samples.
- **Time and Cost Savings:** By eliminating the need for pristine calibrations and reducing the risk of misidentification, AutoRIX saves valuable time and resources.
- **Improved 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, making AutoRIX accessible to users of all levels.

Conclusion

AutoRIX represents a significant advancement in GC/MS analysis. By overcoming the challenges of impure calibrations, scientists are empowered to achieve more accurate and reliable compound identification. This translates to increased confidence in results, streamlined workflows, and ultimately, more impactful scientific discoveries.

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