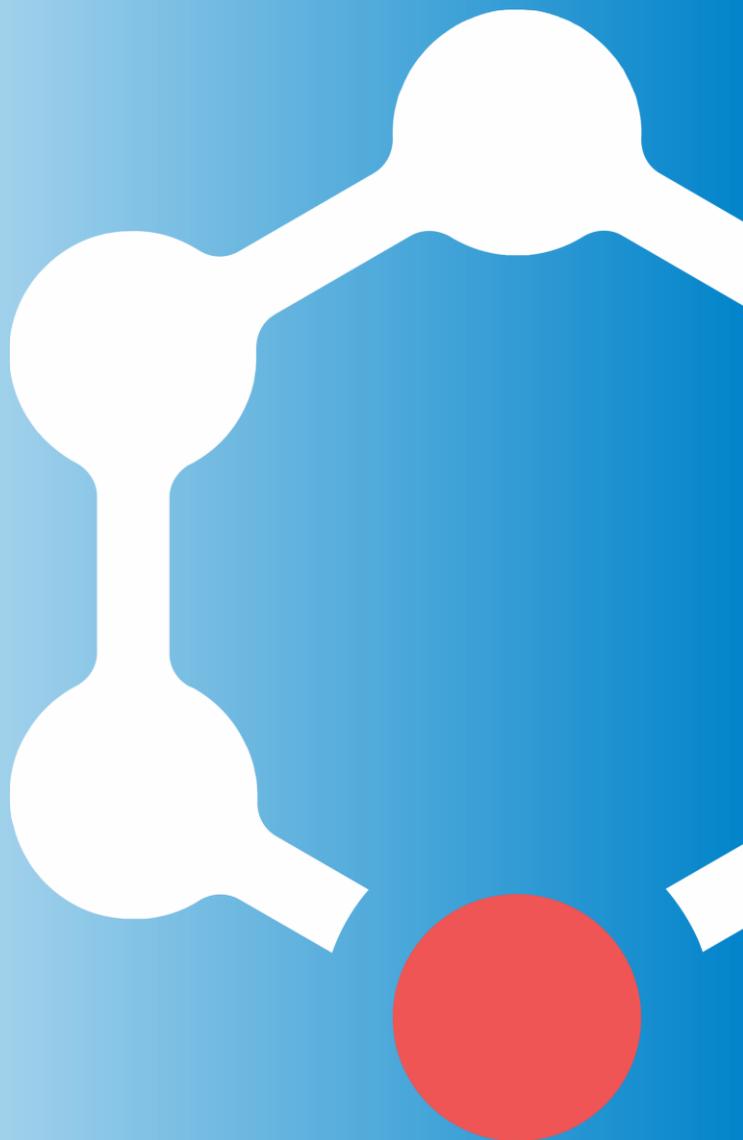




BrightSpec



Structure &
Quantitation,
Simplified



Structural Certainty Without Compromise

BrightSpec's molecular rotational resonance (MRR) platform delivers direct, structure-specific identification and quantitation of small molecules, without chromatography, physical reference standards, or indirect inference.

By measuring gas-phase rotational spectra, MRR provides a molecule's unique three-dimensional fingerprint, enabling chemists to distinguish closely related isomers, confirm stereochemistry, and quantify volatile compounds with confidence.



Compute with BrightHub

Simulation as a Standard

MRR enables structure identification even when reference materials are impossible. BrightHub provides the simulated rotational spectra of three-dimensional molecular structure enabling a novel structure confirmation methodology.

BrightHub, BrightSpec's proprietary simulation software, provides a simple standardized method for simulating rotational spectra. No expertise required, just import the results from BrightHub and go.

Suitability for MRR

Name: Limonene (4-) ✓ Suitable for MRR

PubChem ID: 445917

Molecular Weight: 136.234

Rotatable bonds: 1

Quadrupolar Nuclei: 0

Level One

Submission Queue

| Action | Queue | Compound Name | Level of Theory | Submission Date | Status | Remaining Time |
|----------------------|-------|---------------|-----------------|-----------------|--------|----------------|
| No results available | | | | | | |

Calculation Results

| Action | Compound Name | Level of Theory | Submission Date | Status | Completion Date |
|--------------------------|-------------------------------|-----------------|------------------|----------|------------------|
| <input type="checkbox"/> | Agopin | Level One | 2024-10-29 13:44 | Finished | 2024-10-29 16:30 |
| <input type="checkbox"/> | 2-Chloro-4-hydroxypyrrolidine | Level One | 2024-08-07 14:27 | Finished | 2024-08-07 14:30 |
| <input type="checkbox"/> | Propylene Glycol | Level One | 2024-04-16 16:42 | Finished | 2024-04-16 17:29 |
| <input type="checkbox"/> | Agopin | Level One | 2024-04-15 15:07 | Finished | 2024-04-15 21:38 |
| <input type="checkbox"/> | Sucrose | Level One | 2024-04-04 19:07 | Finished | 2024-04-09 09:33 |
| <input type="checkbox"/> | Agopin | Level Two | 2024-04-04 19:04 | Finished | 2024-04-04 21:35 |
| <input type="checkbox"/> | Agopin | Level One | 2024-01-11 14:32 | Finished | 2024-02-09 01:20 |

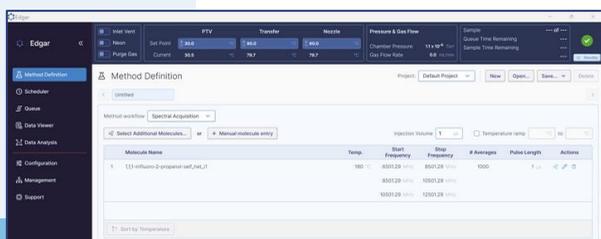
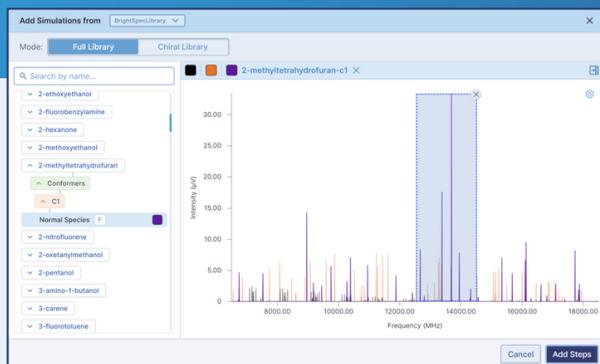


Solve with Edgar

From Simulation to Spectra with Ease

Edgar, our acquisition and analysis software, then takes you from simulation to results in your sample with just a few clicks. Edgar automates method development, sample analysis and spectral fitting, which makes MRR a truly scalable solution for modern analytical chemistry.

Whether working from a new structure identification or BrightSpec's proprietary libraries Edgar provides comprehensive workflows to solve your analytical challenges.



Meet the **spectraMRR**

Comprehensive Quantitation & Confident Structural ID

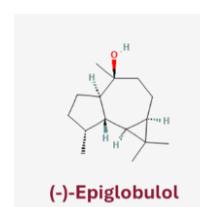
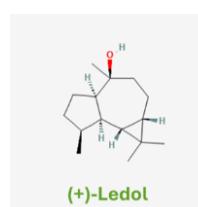
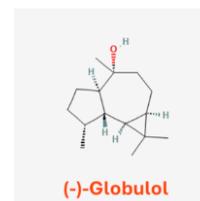
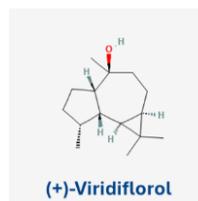
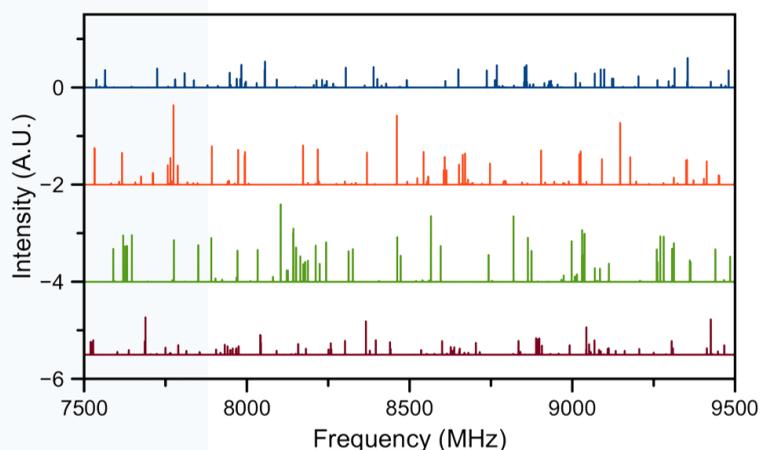
Scientists working with complex mixtures or unknowns often lack a single, simple workflow that enables confident structural identification and quantitative analysis.

Our most powerful system, the spectraMRR, enables unambiguous structure assignment alongside mixture-compatible quantitation. Whether you're solving analytical puzzles or validating synthesis outcomes, spectraMRR gives you absolute confidence in your data—all in a scalable, user-friendly workflow.



- Structure ID & Chiral Analysis
- Full Quantitation & Library Building
- BrightHub Quantum Chemistry Pipeline

Pharmaceutical • Chemical • Consumer Goods



Structure-specific MRR spectra of stereoisomers with identical formulas. Differences in three-dimensional geometry give rise to distinct rotational fingerprints that enable direct discrimination without separation or reference standards.

Meet the isoMRR

Ultra-Precise Quantitation and Chiral Analysis, Streamlined

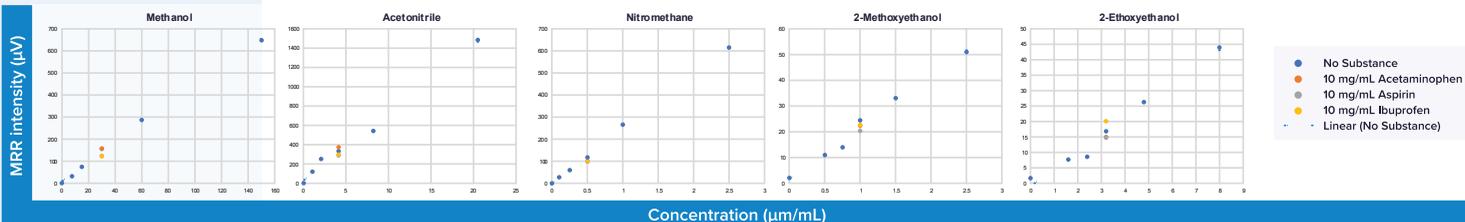
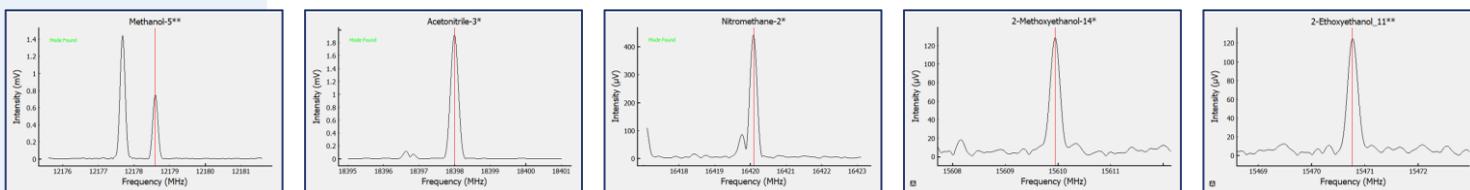
Analytical labs face growing pressure to achieve fast, accurate chemical quantitation and chiral analysis, but the complexity of traditional workflows slows them down.

The isoMRR enables robust, highly specific chemical quantitation. Built on the simplicity of MRR, the isoMRR platform adds advanced quantification capabilities across an array of chemical classes, making it ideal for QA/QC, and process optimization. It's the perfect balance of performance and ease of use for busy analytical labs.



- Chiral Ratios
- Full Quantitation & Library Building
- BrightHub Quantum Chemistry Pipeline

Pharmaceutical • Chemical • Consumer Goods



Structure-specific rotational spectra distinguish individual residual solvents, while consistent signal response versus concentration supports accurate, separation-free quantitation using isoMRR.

Meet the nanoMRR

The Compact Solution for High-Precision Molecular Analysis.

Measuring small, highly volatile molecules like formaldehyde is analytically challenging. Traditional methods often rely on derivatization, indirect detection, or complex sample preparation, introducing uncertainty, time, and operational burden.

The nanoMRR brings the core power of MRR into a compact, accessible platform designed for targeted applications. By directly measuring structure-specific rotational signatures, nanoMRR enables confident detection and quantitation of small, volatile molecules in complex matrices without chromatography or reference standards.

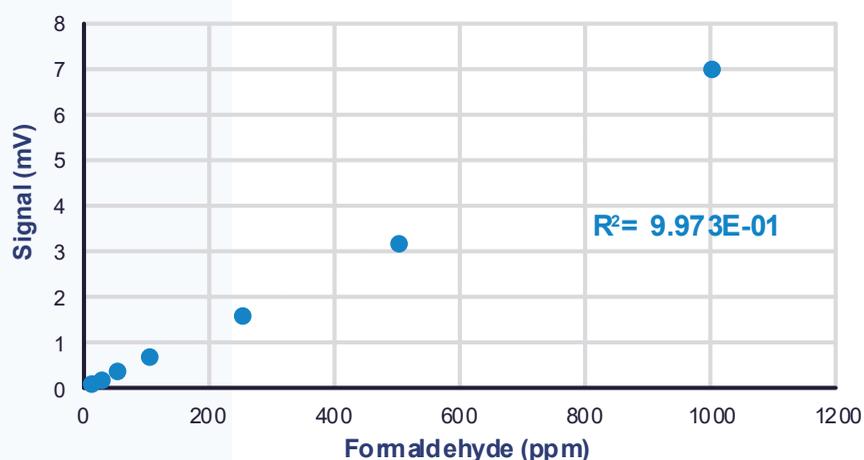
The nanoMRR leverages a pre-built library and does not require BrightHub to operate



- **Quantitation of Key Analytes**

Pharmaceutical • Chemical • Consumer Goods

Formaldehyde Dose Response

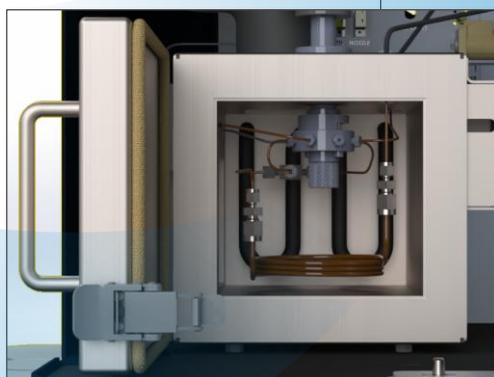


The nanoMRR offers a powerful and flexible solution for formaldehyde detection, delivering a linear response from 15 ppm to 1000 ppm with direct sample injection, streamlining workflows and minimizing operational complexity. The nanoMRR redefines how formaldehyde is quantified.

Why SpectrAline™

SpectrAline™ Cartridges represent a new portfolio of precision-engineered consumables developed through a strategic technical collaboration between BrightSpec, pioneers in Molecular Rotational Resonance (MRR) spectroscopy, and Restek, global leaders in column technology.

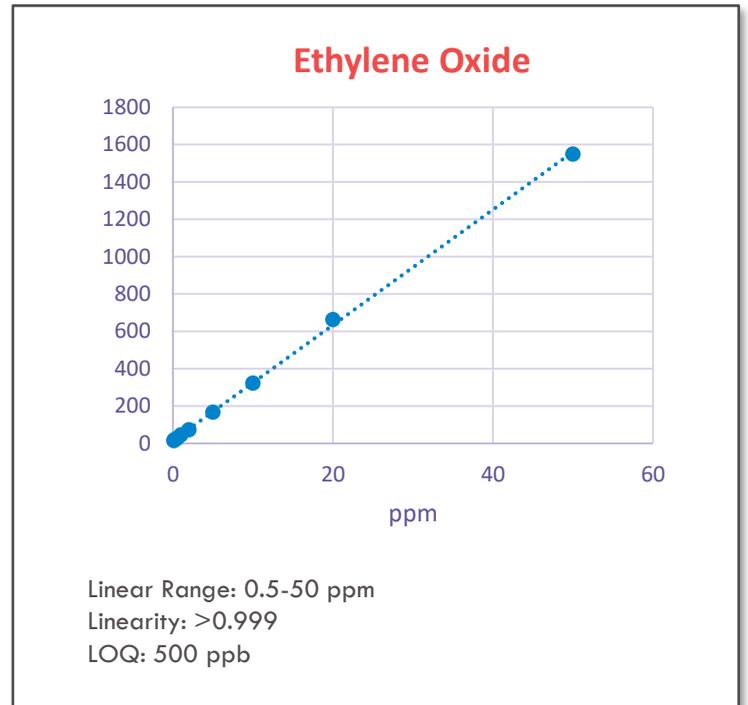
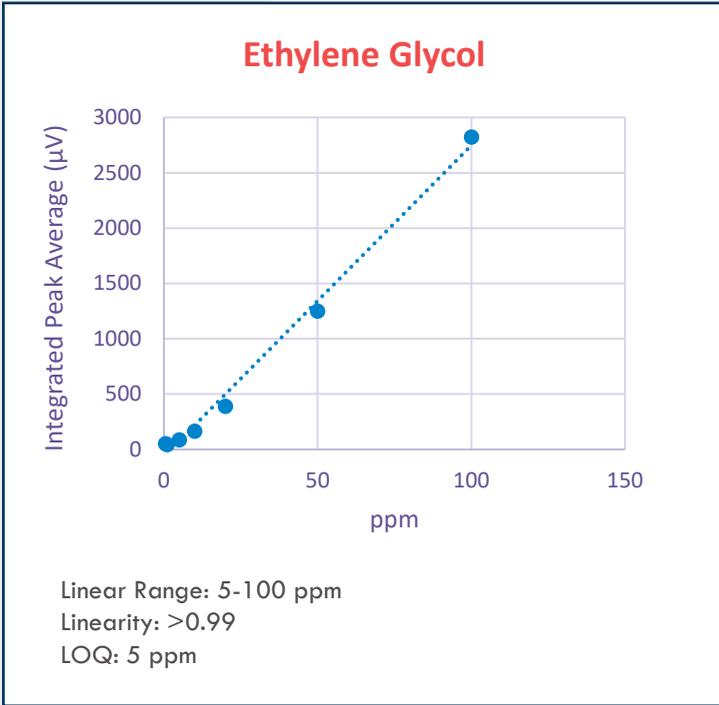
Purpose-built for the spectraMRR™ and isoMRR™ platforms, SpectrAline Cartridges redefine sample introduction for MRR—enhancing the capture, concentration, and controlled transfer of volatile and compounds into the measurement region.



Combining Restek's expertise in the selective capture of volatiles with BrightSpec's structure-specific (MRR) detection, SpectrAline™ Cartridges enable:

- **Higher Sensitivity Where It Matters**
- **Expanded Matrix Compatibility**
- **Simplified Workflows**

Applications



Quantitation and molecular ID simplified.

MRR's unique molecular specificity plus SpectrAline™ cartridges enable challenging analytes to be quantified in complex matrices, no derivatization or ambiguous results.



Food & Authenticity



VOC's



Impurity Analysis



Structure Identification

Our BrightSpec MRR Product Family consists of three instruments with different strengths and target applications. Chemists across academia, pharmaceutical, chemical and consumers goods companies rely on BrightSpec MRR to identify and quantity molecules in complex mixtures in a fraction of the time of their existing workflows.

| Specs | nanoMRR | isoMRR | spectraMRR |
|------------------------|----------|-------------------|-------------------|
| Mass Range | <150 AMU | 50 to 300 AMU | 50 to 300 AMU |
| Sampling | Liquid | Liquid, Headspace | Liquid, Headspace |
| Carrier Gas | None | Neon | Neon |
| Purge Gas | None | Nitrogen | Nitrogen |
| Reference Library | Limited | Full | Full |
| Chiral Analysis | No | Yes | Yes |
| Structure Analysis | No | No | Yes |
| SpectrAline Compatible | No | Yes | Yes |



Learn how MRR can power your chemistry

BrightSpec

Get In Touch:

