BrightSpec

Introducing the

spectraMRR

One easy-to-use instrument to streamline structure identification and quantitation workflows.

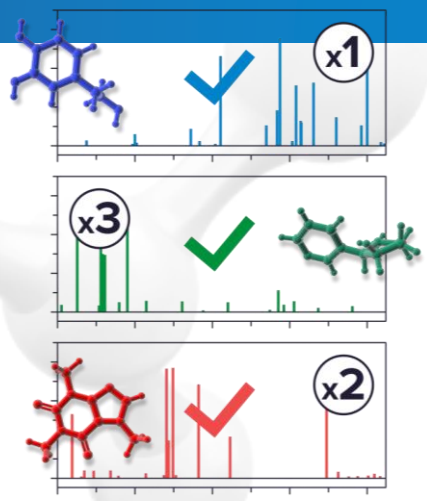
BrightSpec

Technology

Molecular Rotational Resonance

Identify and Quantify Small Molecules
in **One Simple Workflow**.

Molecular rotational resonance (MRR) enables direct, structure-specific identification and quantitation of small molecules, without chromatography, physical reference standards, or indirect inference. BrightSpec's spectraMRR™ instrument offers both ID and quantitation together in a single workflow.



Theoretical Spectra

Instrument

Meet the spectraMRR

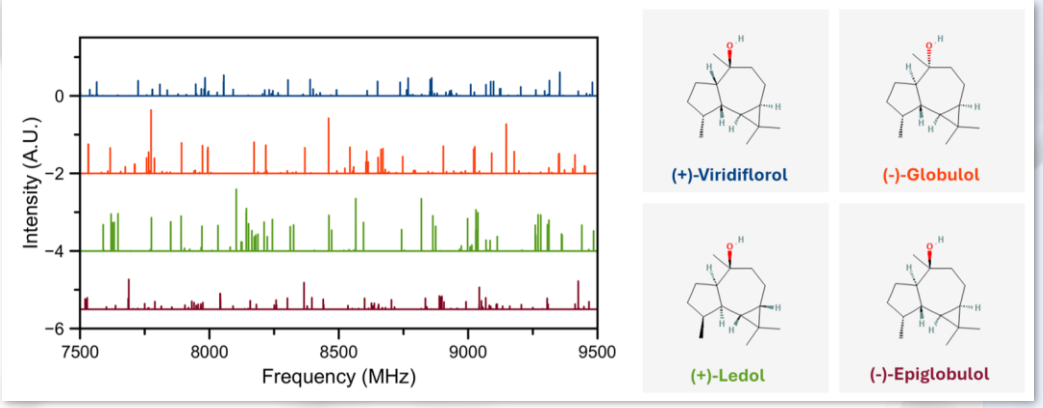
Comprehensive Quantitation & Confident Structure Identification

Our most powerful system, spectraMRR™, enables unambiguous structure assignment, quantitation in complex mixtures and enantiomeric excess (ee) from library molecules. Whether you're solving analytical challenges or validating synthesis outcomes, spectraMRR™ delivers confident, reliable data within a scalable, user-friendly workflow.

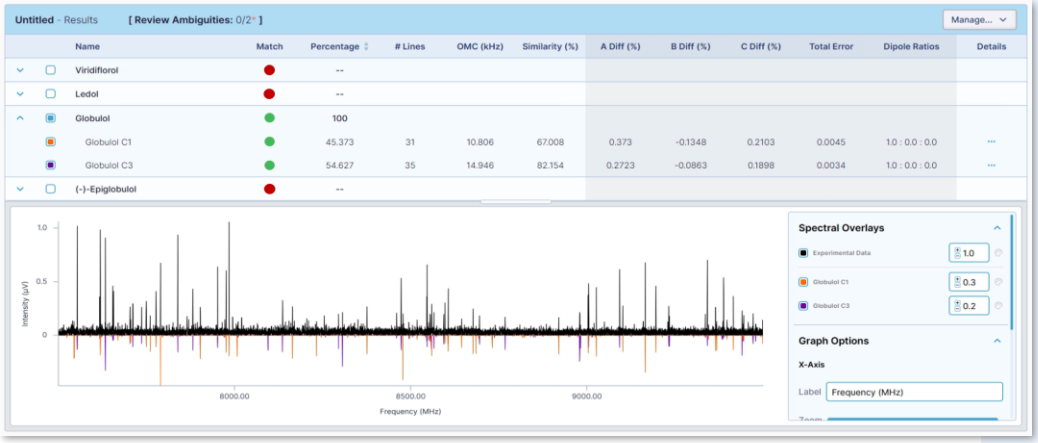
Pharmaceutical • Chemical • Consumer Goods

Structure Identification without Pure Standards

MRR solves structure problems without reference standards or chromatography. This sample was first thought to be viridiflorol, but spectraMRR revealed otherwise. The experimental spectrum did not match viridiflorol, so the team expanded the search to four closely related stereoisomers in BrightHub. Because MRR is sensitive to three-dimensional structure, each candidate gave a unique spectral fingerprint.



- Simulated rotational spectra of closely related sesquiterpene stereoisomers show distinct, non-overlapping spectral fingerprints despite identical molecular formulas and highly similar structures.

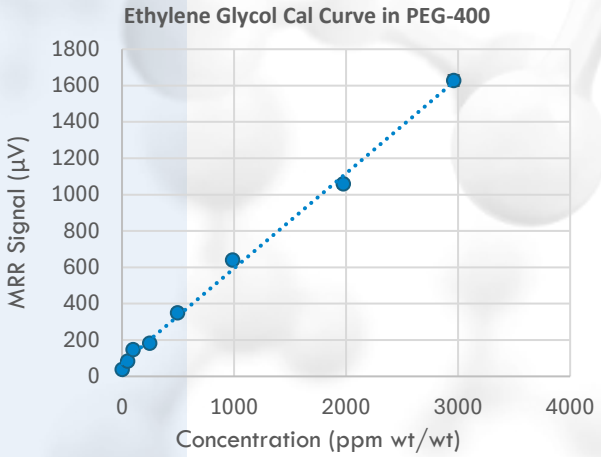


- The spectraMRR can tell apart closely related stereoisomers, giving labs an easier way to confirm difficult structures without pure standards, complex separations, or extensive NMR work.

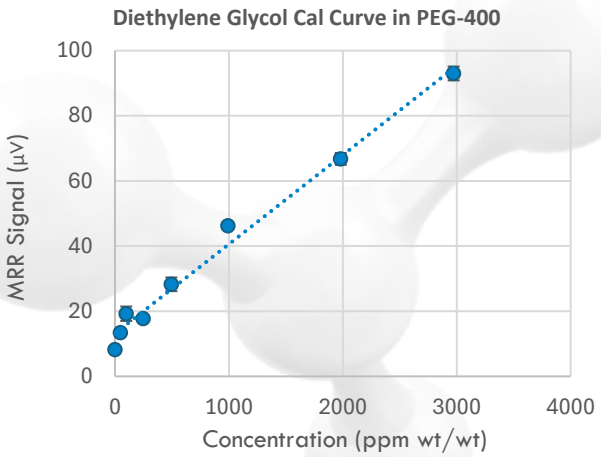
Quantitative Confidence in Challenging Excipient Workflows…

From toxic glycols in PEG-400 to volatile residuals in PEG-3350, the spectraMRR offers a singular solution to traditionally complex multi-step analyses.

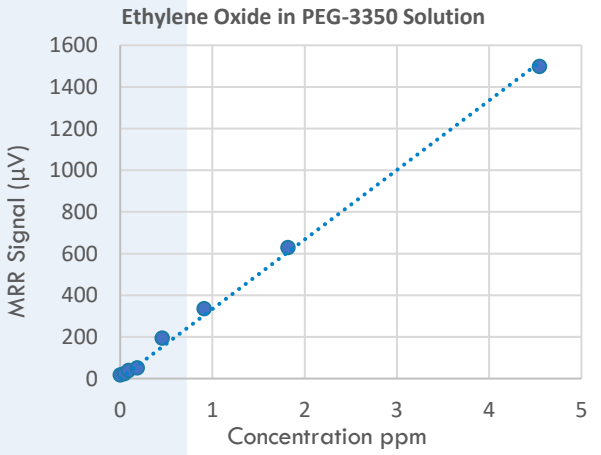
These two application workflows show the same outcome in different matrices: clear linear response, trace-level sensitivity, and confident quantitation with minimal sample handling.



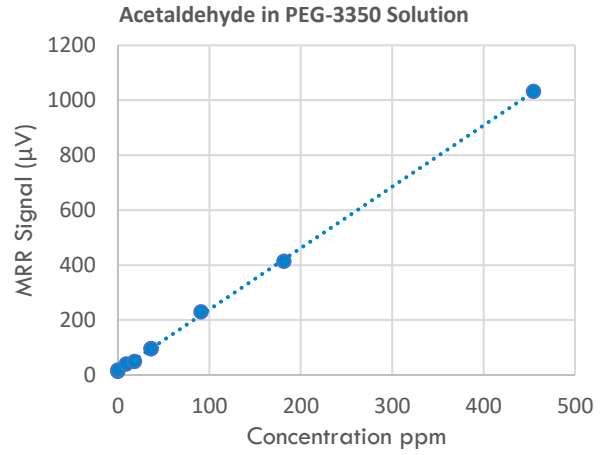
Linear response from 10–2960 ppm with R^2 = 0.9967; LOQ = 10 ppm.



Linear response from 182–2973 ppm with R^2 = 0.9868; LOQ = 182 ppm.



Strong calibration across 0.05–5.0 µg/mL with R^2 = 0.9985; reaches USP-relevant LOQ in ~60 sec.

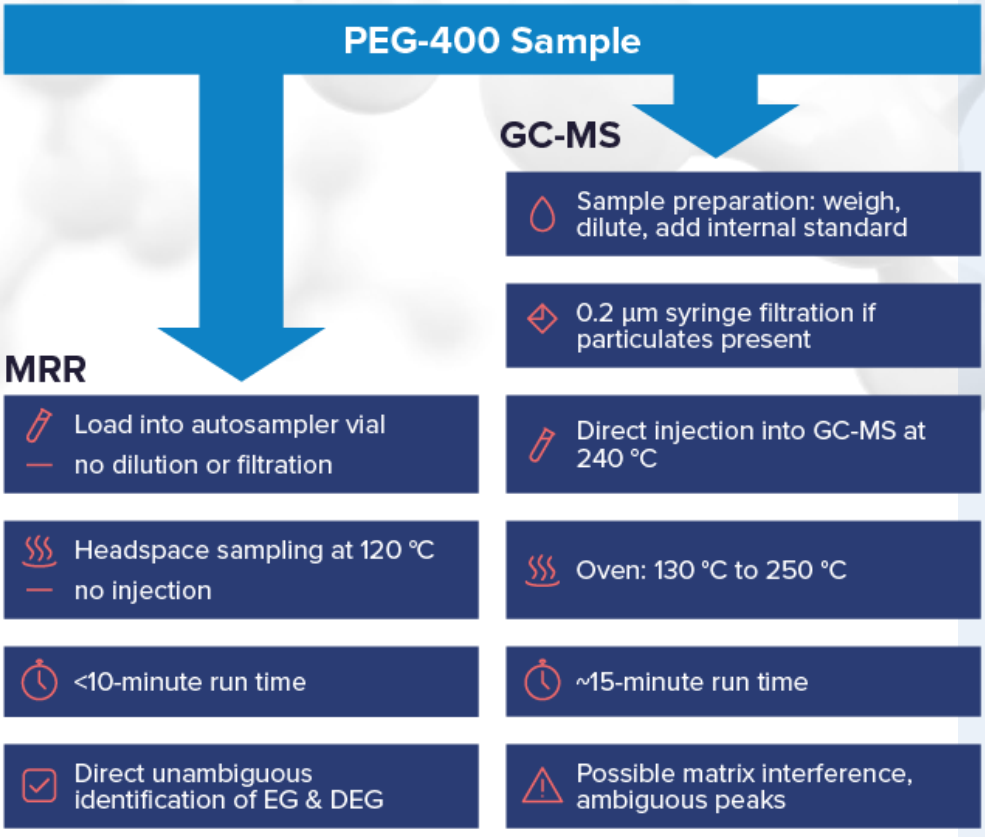


Strong calibration across 10–500 µg/mL with R^2 = 0.9997; reaches USP-relevant LOQ in ~40 sec.

… Without the Usual Bottlenecks

Traditional GC-MS methods can meet regulatory requirements, but in excipient testing they often introduce bottlenecks—from extensive sample prep to matrix-specific method development and slower, more complex workflows.

The spectraMRR simplifies the process with automated headspace sampling and direct molecular identification, enabling minimal sample prep and quantitation in seconds to minutes. In PEG-400 workflows, MRR reduced analysis time by ~75% versus traditional GC methods while maintaining the sensitivity and linearity needed for excipient safety testing.



Key benefits across both workflows:

- ~75% faster analysis in PEG-400
- Minimal sample preparation
- Less method complexity in challenging PEG matrices
- Quantitative confidence for excipient safety testing

Structural Certainty **Without Compromise**

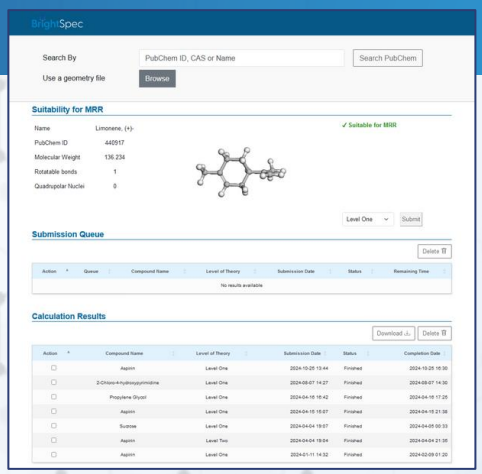
BrightSpec's molecular rotational resonance (MRR) platform delivers direct, structure-specific identification and quantitation of small molecules, without chromatography, physical reference standards, or indirect inference.

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.

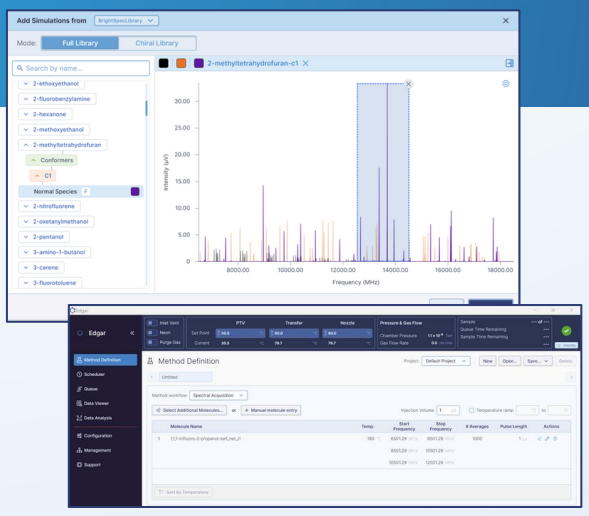
Compute with BrightHub

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. The spectraMRR offers full library building capabilities through BrightHub.



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.

Key Benefits

The spectraMRR™ Advantage

Forget complex methods and incomplete results.
Precision made simple.

Unambiguous Structure

MRR spectra are highly specific to the three-dimensional structure of molecules in the gas phase, allowing you to quantify structures with confidence, even when molecules exhibit isomerism or chirality.

Simplified Methods

Our simplified and easy to optimize workflows also ensure that your methods are robust and transferable, avoiding costly redevelopment and delays.

Streamlined Workflow

MRR provides structural identification and quantitation in a single measurement in mixtures, eliminating the need for sample prep, columns and multiple techniques.

Time Savings

Eliminate the inefficiencies of traditional analytical methods that demand excessive time for sample preparation, method optimization, and manual
data analysis.

spectraMRR

	Technical Specifications	
	Broadband	**Targeted**
spectraMRR Frequency Range	4-18 GHz	6-18 GHz
Acquisition Bandwidth	2 GHz	1 MHz
Liquid Injection Temperature Range	RT+5-200°C	
Headspace Injection Temperature Range	40-200°C	
Instrument Weight	800 lbs	
Instrument Footprint	67" L x 37" W x 72" H	
NA Power Supply	120V, 60Hz, 20A	
EU Power Supply	230V, 50Hz, 16A	
Carrier Gas	Neon (40 mL/ Min.)	
Purge Gas	Nitrogen (Purge)	
Certifications	CE	

Analytical Specs

	Quantitation	Structure
Sample Type	Liquid, Headspace	
Mass Range	50-300 AMU	
Dipole Moment	>0.1 debye	
Liquid Injection Volume	10 µL (Typical)	
Headspace Source Volume	1 mL (Typical)	
Analyte (Typically Required)	100 ng	2 mg
Time to Result (Typical)	<10 Min.	30 Min.
Dynamic Range	> 1:1,000	1:100
Sensitivity (LOQ)	0.001% / ppm	1%
Repeatability	<10% RSD	-
Linearity	R2 >0.99	-
Reference Library (Measured)	>500 Compounds	Library building
Chiral Analysis	%EE	-

BrightSpec