



Introducing the
spectraMRR



Providing simple, precise chemical analysis for leading pharmaceutical, chemical and consumer goods companies around the world.

Spring 2025

Meet the spectraMRR

Structure Analysis Simplified.



The spectraMRR is a cutting-edge analytical platform that harnesses the power of rotational spectroscopy to offer a novel method for the identification of chemical structures, complementing traditional spectroscopic techniques such as NMR, IR, and mass spectrometry.

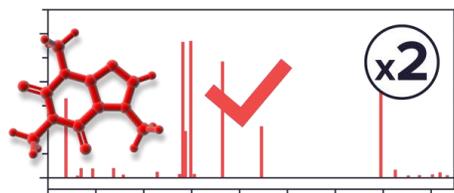
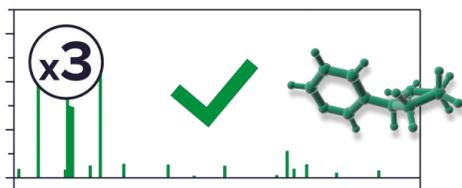
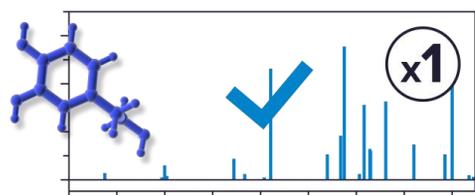
By delivering high-resolution data that can distinguish between even the most subtle structural variations, the spectraMRR enhances confidence in structural analysis and provides unique structural analysis.

Ideal for pharmaceutical and fine chemical development, this platform enables scientists across industries to achieve a deeper understanding of the molecular structures involved in their products and processes.

Technology

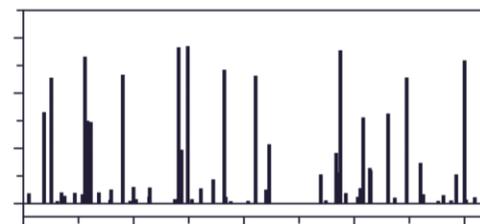
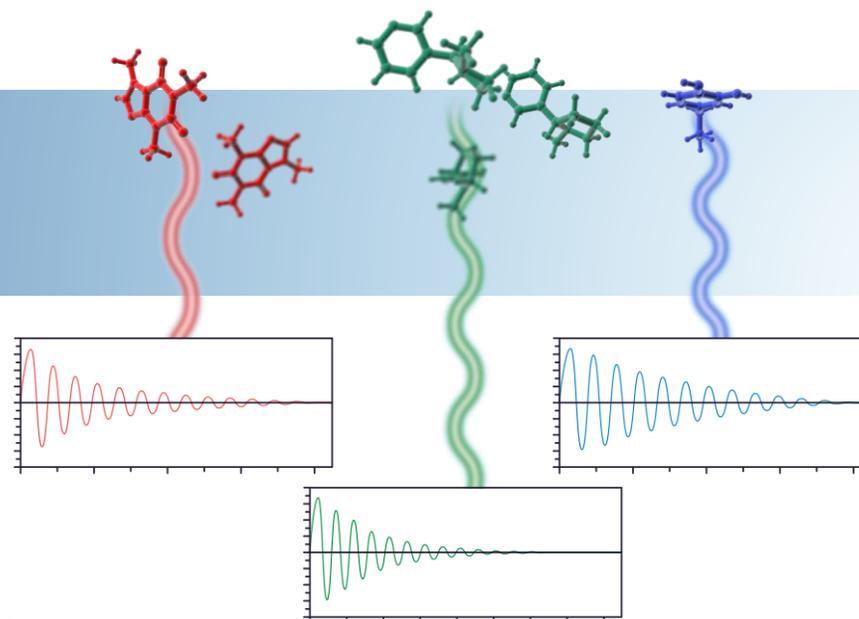
About BrightSpec MRR

Rotational spectra provide unique fingerprints for small molecules in the gas-phase.



Theoretical Spectra

Our instruments utilize MRR technology and microwave-wave radiation to excite molecular rotational transitions, which can then be measured and analyzed to determine the molecular structure and quantify the analyte of interest.



Measured Spectra

BrightSpec is currently the only company commercializing MRR technology and is the global leader in MRR instrumentation. These instruments can be used for a variety of applications that broadly fall in the use cases of reaction optimization, structure validation and targeted quantitation.

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 measure structures with confidence, even when molecules exhibit isomerism or chirality.



Simplified Method Transfer

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.

Compute with BrightHub

A Unique Digital Reference

Simulation as a Standard

MRR enables structure identification even when reference materials are impossible. Rotational spectra can be predicted through the quantum chemistry simulation of three dimensional molecular structure enabling a novel structure confirmation methodology.

No Expertise Required

The spectraMRR platform is supported by BrightHub, BrightSpec's proprietary quantum chemistry pipeline. BrightHub provides a simple standardized method for simulating rotational spectra. No expertise required, just import the results from BrightHub and go.

The screenshot displays the BrightSpec web interface. At the top, there are search options: 'Search By' with a text input for 'PubChem ID, CAS or Name' and a 'Search PubChem' button, and 'Use a geometry file' with a 'Browse' button. Below this is the 'Suitability for MRR' section, which shows the name 'Limonene, (+)', PubChem ID '440917', Molecular Weight '136.234', Rotatable bonds '1', and Quadrupolar Nuclei '0'. A 3D ball-and-stick model of the Limonene molecule is shown to the right. A green checkmark indicates 'Suitable for MRR'. Below this is the 'Submission Queue' section, which is currently empty with the message 'No results available'. At the bottom is the 'Calculation Results' section, which contains a table with columns for Action, Compound Name, Level of Theory, Submission Date, Status, and Completion Date. The table lists several completed calculations for compounds like Aspirin, 2-Chloro-4-hydroxypyrimidine, Propylene Glycol, and Sucrose.

Action	Compound Name	Level of Theory	Submission Date	Status	Completion Date
<input type="checkbox"/>	Aspirin	Level One	2024-10-25 13:44	Finished	2024-10-25 16:30
<input type="checkbox"/>	2-Chloro-4-hydroxypyrimidine	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 17:25
<input type="checkbox"/>	Aspirin	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	2024-04-05 00:33
<input type="checkbox"/>	Aspirin	Level Two	2024-04-04 19:04	Finished	2024-04-04 21:35
<input type="checkbox"/>	Aspirin	Level One	2024-01-11 14:52	Finished	2024-02-09 01:20



MRR's unique digital standard delivers molecular structure in complex samples without reference materials.

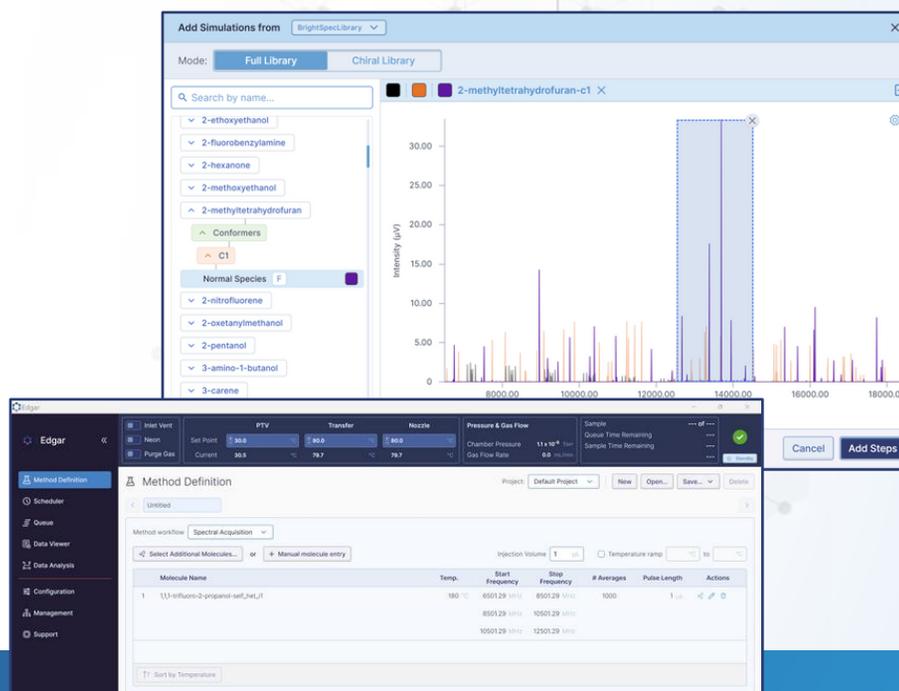
Run with Edgar

From Simulation to Spectra with Ease

Simulation as a Standard

Edgar then takes you from simulation to results in your sample with just a few clicks. After importing the quantum chemistry simulation Edgar selects the optimal spectral region for analysis.

Then a method is optimized based on the molecule's properties and a spectrum is acquired by the instrument.



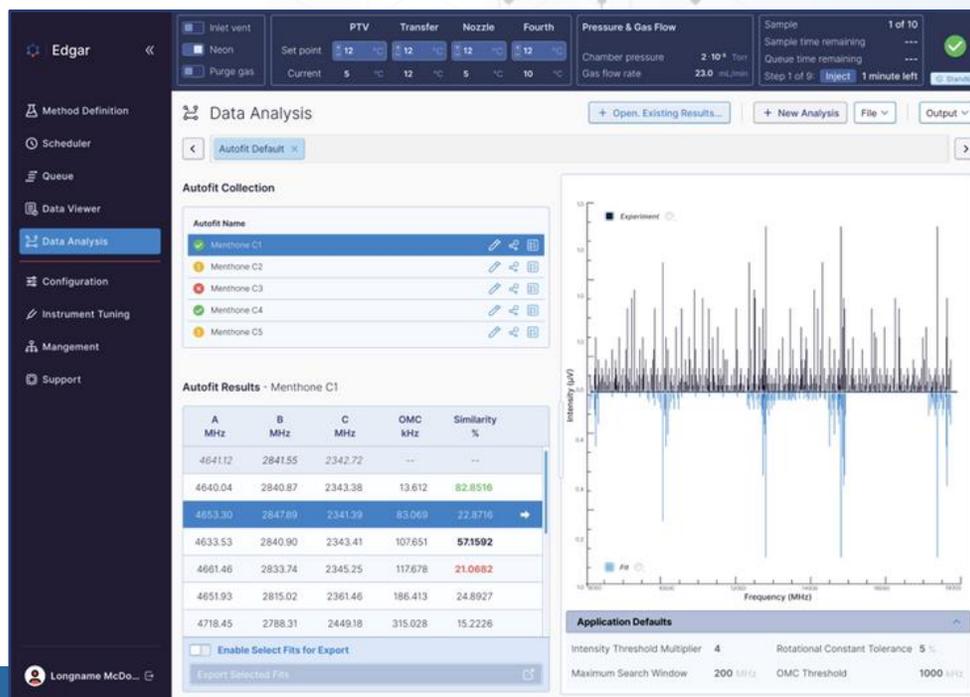
Edgar's intuitive workflows allow you to focus on your science and not method development.

Confirm with Confidence

From Spectra to Solutions in Seconds

Molecular Structure Solved

Finally the simulation and the acquired spectra are compared to confirm the identity of the molecule. Fits from rotational spectra are unambiguous and once confirmed the frequencies can be added to a library and measured on any BrightSpec instrument.



MRR's unique spectral signature provides the ultimate confidence in your structural assignment.

Automated Library Building

Rapidly Generate Spectral Libraries

Setup Batch

Load Samples

Start

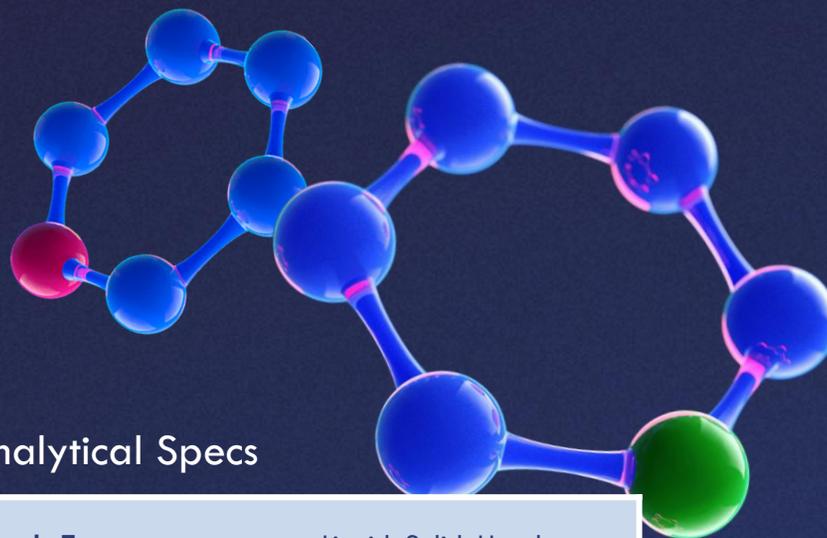
View Results

Our spectral analysis capabilities are built for scale. Acquiring rotational spectra have been extremely time consuming due to manual requirements. Now, chemists can build vast reference libraries using a simple, automated workflow.



Automated workflows and batch processing allow you to scale your work to the next level.

Specifications



Instrument Specs

Frequency Range	6-18 GHz
Liquid Temperature Range	RT-300C
Headspace Temperature Range	RT-200C
Weight	800 lbs
Footprint	67" L x 37" W x 72" H
Power Supply	120V 15A
Carrier Gas	Neon
Certifications	CE

Analytical Specs

Sample Type	Liquid, Solid, Headspace
Materials Required (Structure)	5 mg
Mass Range	50-300 AMU
Dipole Moment	>0.1 debye
Time to Result	1 Hour
Reference Library	500 Compounds
Chiral Analysis	Yes
Structure Analysis	Yes