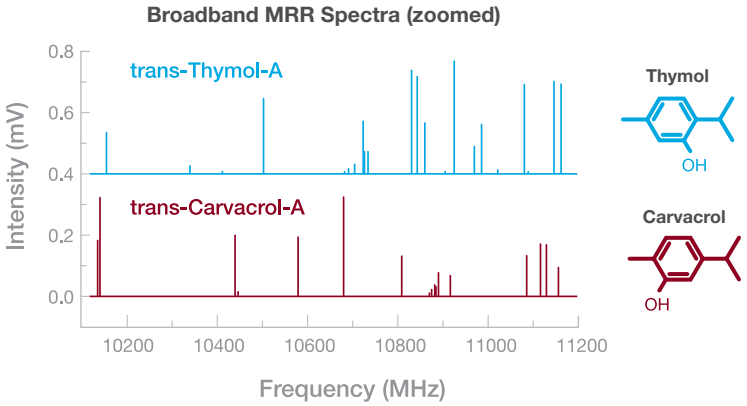
Unambiguous Molecular Identification and Quantification

Molecular Rotational Resonance (MRR) simultaneously provides unambiguous identification and quantification of small molecules by measuring their unique spectral fingerprint.

MRR's chemical specificity easily discriminates between all types of isomers including regioisomers (shown in figure below), diastereomers, enantiomers (providing EE and AC), and isotopic species with site-specific information.

Structural Validation

MRR identifies molecules through the characterization of their rotational spectra, where subtle differences in structure produce significant changes in their spectra. Quantum chemistry calculations allow for the unambiguous confirmation of the molecular identity, without a pure reference standard.



Routine Analysis

High sample throughput is achieved by the speed of MRR analysis with minimal sample preparation.

Additionally the high resolution, sensitivity, and specificity of MRR eliminates the need for front-end separation allowing for the direct analysis of complex mixtures, enabling online reaction monitoring.

Quantitation is achieved without reference standards as the signal is directly proportional to the sample concentration.

Several recent publication provide deeper insight into the utility of MRR:

Chiral Analysis of Linalool, an Important Natural Fragrance and Flavor Compound, by Molecular Rotational Resonance Spectroscopy
BrightSpec (Sonstrom, Cannon, Neil): Symmetry, 2022, 14, 917 **[OPEN ACCESS]**

Chiral Analysis of Pantolactone with Molecular Rotational Resonance Spectroscopy
BASF, Pate and co-workers: Chirality, 2022, 34, 114-135 **[OPEN ACCESS]**

Direct regioisomer analysis of crude reaction mixtures via molecular rotational resonance (MRR) spectroscopy
Merck, Pate and co-workers: Chem. Sci., 2020, 11, 6332-6338

Rapid quantification of isomeric and dehalogenated impurities in pharmaceutical raw materials using MRR spectroscopy
GSK, Pate and co-workers: Journal of Pharmaceutical and Biomedical Analysi, 2020, 10, 113474

BrightSpec Product Portfolio

BrightSpec offers a complete line of MRR spectrometers. The Broadband MRR delivers comprehensive sample profiling and characterization of molecular structures, including new compounds, without a reference standard.

The isoMRR provides routine analysis, screening and quantitation, and direct chiral or achiral process monitoring.

Additionally, BrightSpec offers a line of MRR spectrometers designed for Educational and Fundamental research. Please reach out for more information on what BrightSpec has to offer.

Broadband MRR

Structural Elucidation and Research

Typical Applications	Structural Elucidation Enantiomeric Excess Quantitative Mixture Analysis
Frequency Range	2–8 GHz, 6–18 GHz
Analyte Range	100–400 amu
Analysis Time	60+ minutes
Sample Type	Solids, Liquids and Gases
Sample Volume	5–50 mg (typical)

*Specifications are sample dependent

isoMRR

Routine and Targeted Analysis

Typical Applications	Isomeric Impurity Quantification Enantiomeric Excess Continuous Process Monitoring
Frequency Range	6–18 GHz
Analyte Range	100–400 amu
Analysis Time	5–20 minutes
Sample Type	Solids, Liquids and Gases
Sample Volume	0.5–5 mg (typical)

*Specifications are sample dependent

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