



Edited By: Roberto R. Gil
Online ISSN: 1097-458X
Print ISSN: 0749-1581
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Latest issue
Volume 64, Issue 9
September 2026

Magnetic Resonance in Chemistry is an analytical chemistry journal for scientists in academia and industry who want to keep up-to-date with the latest practical applications of magnetic resonance techniques.

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Issue Information

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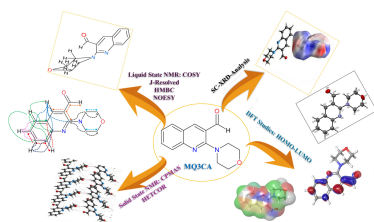
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A Synergistic Approach to the Structural Characterization of 2-(Morpholin-4-yl)quinoline-3-carbaldehyde by Solution and Solid-State NMR Spectroscopy, Supported by Single-Crystal X-Ray Diffraction and DFT Calculations

Srinivasa, Nivedita R. Desai, P. A. Suchetan, Swamy Sreenivasa, Tadimety Madhu Chakrapani Rao, Shivakumar, Udayakumar Dalimba, D. B. Aruna Kumar

First Published: 31 July 2026

Graphical Abstract



An integrated solution- and solid-state NMR approach, supported by single-crystal X-ray diffraction and DFT calculations, enabled comprehensive structural characterization of 2-(morpholin-4-yl)quinoline-3-carbaldehyde (MQ3CA). Multidimensional NMR established complete resonance assignments, whereas crystallographic and computational analyses revealed molecular conformation, crystal packing, and electronic structure.

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Validation of ERETIC-Based ¹H-NMR for the Simultaneous Quantification of Cannabinoids in Complex *Cannabis sativa* Extracts

Rocío Figueroa, Federico Arrighi, Mauricio Cattaneo, Miguel Gilabert

First Published: 23 July 2026

Graphical Abstract

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