

# Comparative Conformational Analysis of IAM and IAA and Related Compounds: Structural Insights into Their Biological Roles

*Wednesday 17 September 2025 12:50 (20 minutes)*

This work presents a comparative rotational spectroscopic study of two biologically relevant indole derivatives: 3-indoleacetic acid (IAA) and indole-3-acetamide (IAM), analyzed using chirped-pulse Fourier transform microwave (LA-CP-FTMW) spectroscopy in the 6–14 GHz frequency range. Based on previous studies focused on the individual structural characterization of serotonin, an important biomolecule, our approach emphasizes a structural and conformational comparison of IAA and IAM with related systems originating from the same precursor. Although these compounds participate in different biosynthetic pathways—IAA and IAM in auxin biosynthesis, and serotonin in neurotransmission—they all share tryptophan as a common biosynthetic precursor. By analyzing their intramolecular interactions, particularly hydrogen bonding, we investigate how these forces influence the conformational landscapes of each molecule. Our results reveal significant differences in conformational preferences and intramolecular stabilization mechanisms, which may be closely related to their distinct biological functions. This comparative approach provides valuable structural insights into how small variations in functional groups can affect the molecular behavior of indole derivatives in biological systems.

## Keywords

indole derivatives, rotational spectroscopy, hydrogen bond, gas-phase

## This abstract is submitted for....

HBond 2025 conference

**Primary authors:** Prof. LEÓN, Iker (Universidad de Valladolid); MUNICIO SAN JOSE, SOFIA (Universidad de Valladolid)

**Co-authors:** Prof. ALONSO, Elena Rita (Universidad de Valladolid); Prof. ALONSO, Jose Luis; Mr MATO, Sergio

**Presenter:** MUNICIO SAN JOSE, SOFIA (Universidad de Valladolid)