THE NICOTINIC-AGONIST CYTISINE: THE ROLE OF THE NH···N INTERACTION [a]

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In this work, we present a comprehensive structural study of cytisine, a potent nicotinic agonist, for which we aim to clarify its bioactivity using high-resolution rotational spectroscopy. In a first step, we used our chirped-pulse spectrometer to characterize two different conformers presenting axial and equatorial arrangements of the piperidine NH group. In sight of the crucial role of the environment of the heteroatoms in cytisine molecule for docking the nicotinic receptor, we used a cavity-based technique to resolve the ^{14}N quadrupole hyperfine structure in a second step. It has allowed us to obtain a detailed structural description of the molecule, clarifying the disposition of the piperidine NH group and further revealing an exotic intramolecular NH···N interaction. This intramolecularity justifies the over-stabilization of the axial conformer over the equatorial form and demonstrates the positive action of this alkaloid on the nicotinic receptor.

[a]ACKNOWLEDGMENTS: THE AUTHORS THANKS THE FINANCIAL FUNDINGS FROM MINISTERIO DE CIENCIA E INNOVACIÓN (GRANTS PID2019-111396GB-I00) AND JUNTA DE CASTILLA Y LEÓN (GRANTS VA244P20).