
ARIAweb: a server for automated NMR structure calculation

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Résumé

Nuclear magnetic resonance (NMR) spectroscopy is a method of choice to study the dynamics and determine the atomic structure of macromolecules in solution. The standalone program ARIA (Ambiguous Restraints for Iterative Assignment) for automated assignment of nuclear Overhauser enhancement (NOE) data and structure calculation is well established in the NMR community. To ultimately provide a perfectly transparent and easy to use service, we designed an online user interface to ARIA with additional functionalities. Data conversion, structure calculation setup and execution, followed by interactive visualization of the generated 3D structures are all integrated in ARIAweb and freely accessible at <https://ariaweb.pasteur.fr>.

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