Journal of Magnetic Resonance

Volume 160, Issue 1, January 2003, Pages 65-73

The Xplor-NIH NMR molecular structure determination package

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https://doi.org/10.1016/S1090-7807(02)00014-9

Abstract

We announce the availability of the Xplor-NIH software package for NMR biomolecular structure determination. This package consists of the pre-existing XPLOR program, along with many NMR-specific extensions developed at the NIH. In addition to many features which have been developed over the last 20 years, the Xplor-NIH package contains an interface with a new programmatic framework written in C++. This interface currently supports the general purpose scripting languages Python and TCL, enabling rapid development of new tools, such as new potential energy terms and new optimization methods. Support for these scripting languages also facilitates interaction with existing external programs for structure analysis, structure manipulation, visualization, and spectral analysis.

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