A General Toolkit for Computation of NMR Properties: Development and Applications

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Interpretation of NMR experiments requires very often the comparison of measured observables against those values computed on 3D models using a variety of algorithms. Commonly, the difference between observed and computed values is included as restraints in a general force-field allowing the use of simulated annealing algorithms. Although a very convenient method for biopolymers, this procedure is generally not well suited for small organic molecules where the local detail, and therefore quality of the forcefield is important. An alternative procedure is the generation of a multiconformer ensemble and determination of Boltzmann populations by fitting the computed NMR observables to the experimental measurements.

In order to facilitate the use of NMR experiments for structure determination of small organic molecules our group started a software development project called **NMRDev** with the intention to build a general and easy-to-use toolkit for the computation of NMR observables from 3D molecular structure. The NMRDev software consists of several object-oriented C++ libraries with a consistent programming interface. This set of libraries allows parsering of most popular chemical file formats, storing and manipulation of molecular properties (geometries, connectivities, populations...) as well as OpenGL based molecular rendering utilities and control over the interaction of rendered objects and the user. These libraries are freely available under the General Public License at http://galileo.usc.es/~armando/software/nmrdev.

Using the NMRDev toolkit we have implemented several modules (plugins), all of them with their own graphical interface embedded in the main NMRDev application:

1. A module for computation of **NOE** intensities using the full-relaxation matrix approach.
2. Computation of alignment tensors using **Residual Dipolar Couplings** and Chemical Shift Anisotropies.
3. A module for computation of **Scalar Coupling Constants** and easy implementation of Karplus-like relationships.

All these modules are distributed in the commercial **MSpin** package (http://www.mestrelab.com) As an example we will present the application of this software to the determination of conformational properties in small organic molecules such as quinine or phenylmenthol.

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