

# ORIEL

Version 1.c, February 2001

## 1. Introduction

ORIEL is the computer program that implements the procedures described in:

M.X. Fernandes, P. Bernadó, M. Pons and J. García de la Torre, "An analytical solution to the problem of orientation of rigid particles by planar obstacles. Application to membrane systems and to the calculation of dipolar couplings in NMR spectroscopy", *Journal of the American Chemical Society*, 123, 12037-12047 (2001).

Please cite this reference in publications of works where ORIEL is employed.

Further information on the theoretical details is available in an Appendix to this article, which is available as Supporting Information from the *Journal of the American Chemical Society* server.

A separate document (postpubli.doc) contains some post-publication notes.

## 2. Purpose and usage

ORIEL calculates the  $^{15}\text{N}$ -H residual dipolar couplings of proteins oriented by bicelles. The program determines the shape of the protein and, eventually, the orientation of the N-H vectors, from its three dimensional structure specified by a PDB file

ORIENL reads a data file named **model.dat.txt** An example of this file is:

```
KH3 protein           !title
KH3_Results.txt      !results
1khm_1.pdb           !input
3.1                   !radius
1                     !iflag
0.03106              !VolFrac
40.                   !Thickness
0.8                   !Scorr
0.85                 !S_LS
```

where

- **title** is a name or title given to the calculation
- **results** is the name of the file that will contain the main results
- **input** is the name of a PDB-formatted file containing the atomic coordinates

- **radius** is the effective radius assigned to the non-hydrogen (extended atoms). Presently we recommend 3.1 Angstroms
- **iflag** can adopt the following values
  - = 1 means that the PDB file does not contain hydrogens. Thus the N-H vectors will be calculated from the molecular geometry
  - =2 means that the PDB file contains explicit hydrogens. Thus the N-H vectors will be calculated from the coordinates of N and H atoms
  - =9 means that the user wants to supply his/her own list of dipoles. In this case, after the iflag line there will be an extra line with the name of the file containing those dipoles. The first line in this file will have the number of dipoles, and the following line the three cartesian coordinates of each of them.
- **VolFrac** is the volume fraction of bicelles (ratio of the volume occupied by the bicelles – determined from their mass concentration and density – and the total volume of the system).
- **Thickness** is the thickness in Angstroms of the bicelles
- **scorr** is an empirical correction factor, introduced by Zweckstetter and Bax (JACS 122, 2791, 2000) to account for imperfect alignment of the bicelles with the magnetic field. Following these authors we employ the value 0.8
- **s\_LS** is the Lipari-Szabo order parameter of the dipole. As a typical value we employ 0.85 for all the residues.

### 3. Notes

- The volume fraction of bicelles, VolFrac, can be obtained from the w/v (weight per volume) concentration using 1.03 g/ml for the bicelle density
- The value taken for the N-H distance is 1.04 Å.

### 4. Last version

Version 1.c contains a minor correction to the previous version (1.a)

### 5. Availability

Executables of the latest version of this program, for various platforms, and related documentation can be obtained from the web site:

<http://leonardo.fcu.um.es/macromol/>

**For comments, suggestions, help... please contact:**

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