

CYANA 2 - Migration from earlier Cyana versions

Hints for a successful and smooth migration from CYANA 1 (and from Dyana) to CYANA 2. A more [detailed list](#) of new features in CYANA 2 is also available.

CYANA 1 features are shown in blue, corresponding CYANA 2 features in red.

- **Installation:** CYANA 2 is written in Fortran 90/95. The recommended compiler on Linux systems is the [Intel](#) Fortran compiler that is available free-of-charge from Intel. The program cannot be compiled with Fortran 77 compilers like GNU's 'g77'.
- **Nomenclature:** The standard residue library of CYANA 2 adheres to strict IUPAC nomenclature for amino acids. Compared to the standard libraries of CYANA 1 and Dyana there are the following changes in atom nomenclature amino acids:

Backbone amide proton: HN --> H

Glycine alpha protons: HA1/HA2 --> HA2/HA3

The most common forms of the amino acid residues are referred to by the standard three-letter code, i.e. there are the following changes for charged residues:

LYS+, ARG+, GLU-, ASP- --> LYS, ARG, GLU, ASP

The straightforward way to convert data files to the new nomenclature is by using Cyana itself. The demos include an example script for this purpose, 'MigrateFromDyanaCyana1.cya'.

If, for some reason it is desirable to continue using the old CYANA 1/Dyana nomenclature together with the new library, this is possible simply by inserting the 'translate dyana' command in the local startup script (./init.cya).

The old CYANA 1/Dyana library is still available and can be loaded with the 'dyanalib' command, whereas 'cyanalib' will load the standard library that is based on the widely used geometric parameters of Engh and Huber (Acta Crystallogr. A47, 392-400, 1991).

- **Larger van der Waals radii:** In order to achieve energetically more favorable structures, the standard library of CYANA 2 uses significantly larger van der Waals radii for the repulsive term of the target function than the standard libraries of CYANA 1 and Dyana. Therefore, target function values will in general be slightly higher than before. This does not mean that the structures have lower quality.
- **Replaced commands:**
 - Automated NOE assignment: candid --> noeassign
 - Reading BMRB chemical shift lists: bmrblast --> read bmrblast
 - CA shift angle restraints: cashifts --> cashiftaco
 - Cis-proline check: cispro --> cisprocheck
 - Ramachandran plot: ramachandran --> ramaplot
 - CA shift plot: caplot --> cashiftplot
- **Changes in combined automated NOE assignment and structure calculation:**
 - NOE assignment files: cycle?.ass --> cycle?.noa
 - Filter NOE assignment files: candidlist --> cyanafilter
 - Overview table: candidtable --> cyanatable

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