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CYANA

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Synonyms

Combined assignment and dynamics algorithm for NMR applications

Definition

CYANA is a software package for the structure calculation of proteins and nucleic acids on the basis of multidimensional NMR data. Three-dimensional structures are calculated by simulated annealing using a fast algorithm for torsion angle dynamics, that is, molecular dynamics simulation with the torsion angles as the only degrees of freedom. The efficiency of the approach results from the elimination of high-frequency bond-stretching and bond-bending motions that allows for much longer integration time steps than conventional Cartesian space molecular dynamics simulation and from the use of a highly simplified "geometric" force field that retains only short-distance interactions. The principal experimental input data are conformational restraints on interatomic distances derived from nuclear Overhauser effect spectroscopy (NOESY). In addition, restraints on torsion angles derived from chemical shifts of scalar coupling constants, hydrogen-bond restraints, residual dipolar couplings, and paramagnetic pseudocontact shifts can be used as input data for structure calculations. CYANA provides an algorithm for combined automated assignment of NOESY cross peaks and protein structure calculation, which has largely replaced the cumbersome and error-prone manual NOESY assignment approach (Güntert and Buchner 2015). In addition, CYANA includes the FLYA algorithm for fully automated NMR protein structure determination that can substitute all manual spectra analysis, including peak picking, resonance assignment, and NOESY assignment, and thus overcomes a major efficiency limitation of the NMR method for protein structure determination (Schmidt and Güntert 2012). Further information on CYANA can be found at http://www.cyana.org.

Cross-References

- ▶ Molecular Dynamics Simulations of Proteins
- ▶ Multidimensional NMR Spectroscopy
- ▶ NMR

G. C. K. Roberts, A. Watts (eds.), *Encyclopedia of Biophysics*,
https://doi.org/10.1007/978-3-642-35943-9_323-1

▶ NMR-Based Structural Proteomics
▶ Nuclear Overhauser Effect
▶ Protein NMR Resonance Assignment

References

Güntert P, Buchner L (2015) Combined automated NOE assignment and structure calculation with CYANA. J Biomol NMR 62:453–471

Schmidt E, Güntert P (2012) A new algorithm for reliable and general NMR resonance assignment. J Am Chem Soc 134:12817–12829