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Protein structure calculation with a max-min ant system

J Gimmler*[1], W Gronwald[2], H Möller[1] and TE Exner[1]

Address: [1]Universität Konstanz, Universitätsstr. 10, 78464 Konstanz, Germany and [2]Universität Regensburg, Josef-Engert-Str. 9, 93053 Regensburg, Germany

* Corresponding author

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Despite the fact that many different programs have been developed in the field of NMR-based structure determination, the 3D structure determination of a large protein is still very time consuming and needs a lot of manual intervention. Therefore, it is highly desired to automate as many of the steps "peak picking", "assignment", and "structure calculation" as possible in a self-consistent manner. To be successful, such programs have to be very flexible to benefit from different types of constraints and robust in dealing with ambiguities and noise in the spectra.

Here, we introduce a new expandable approach to determine the 3D structure of proteins. At the moment this includes the final step of structure calculation from distance as well as angle constraints. A special kind of Ant Colony Optimization algorithm, namely a Max-Min Ant System [1] (MMAS) is used to optimize the protein conformation in torsion angle space. The structure is optimized with respect to a target function that scores the different conformations taking constraint violations into account.

New developments aim at considering highly ambiguous distance constraints, which are obtained from automatic NOE assignments. To cope with these ambiguous distance constraints we use different approaches, especially probabilities for possible assignments calculated with the program KNOWNOE [2] to guide the search.

References

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