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Algorithms for analysis of NMR projections: Design, implementation and applications

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Akademisk avhandling för filosofie doktorsexamen i Naturvetenskap, som med tillstånd från Naturvetenskapliga fakulteten kommer att offentligt försvaras onsdagen den 20 april 2011 kl. 14:00 i KS101, Institutionen för kemi, Kemigården 4, Göteborg.

ISBN: 978-91-628-8277-8

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Abstract

With an increasing rate of protein expressions the need for fast protein characterization has become more important. Protein NMR has long been an important contributor for protein characterization; being one of a few techniques that can study proteins at atomic resolution in their native state. Whitin recent years faster experimental and processing methods have emerged that are now becoming routine. This thesis describes algorithms for automatic backbone assignment and validation of structure information by using projection experiments together with a decomposition method. Projection experiments reduce measurement time for multidimensional spectra thus making it possible to obtain very high dimensional spectral information in a fraction of the time required for a conventional experiment. By combining different experiments backbone, side chain and NOE information can be obtained. A set of software tools for automatic backbone characterization where developed from the implementation of different algorithms in conjunction with different proteins and projection experiments. Testing and refinement of the different tools resulted in a robust characterization method well suited for different proteins. Possible future projects are expanding the methods to side chain and structure determination making the characterization more complete.

KEYWORDS: NMR, projection experiments, decomposition, algorithm, automatic assignment, proteins, NOESY, reduced dimensionality, peak picking.

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