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Full-automated Structure Determination Approach for Structural Proteomics

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Structural proteomics has been considered as an important research area for post-genomics era. However, the speed for high-throughput protein structure determination requires more fast and efficient technical methodology that includes new experimental techniques and automation for data manipulation. In this study, automation methods that have been developed by many frontier labs were integrated and tested for two small proteins. HP0371 derived from *Helicobactor pylori* and MTH1880 from *Methanobacterium Thermoautotrophicum* were used as test examples. For high-throughput structure determination, automatic assignment of NMR data was performed with minimal NMR data set including 15N edited NOESY and TOCSY, HNCACB, CBCA(CO)NH, HNHA, 13C edited HMQC-NOESY and HCCH-TOCSY. Backbone assignment was successfully made with AUTOASSIGN and AUTOPEAK program. NOEs generated by SPARKY analysis were used as an input data for structure calculation with both CYANA and ARIA and two independent results were compared. Both programs were implemented to Linux cluster system with MPI and remote shell. Finally, the quality of the integrated automatic tools will be discussed by comparison with data from traditional manual prodedure.