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1. Definition of the Software

UNIO is a software package for automated NMR data analysis. It provides the functionalities of the four existing algorithms: MATCH, for automated backbone assignment, ASCAN, for automated side-chain assignment, ATNOS, for automated peak picking and NOE identification in 2D homonuclear and 3D heteronuclear-resolved NOESY spectra, and CANDID, for automated NOE assignment of NOESY cross peaks in conjunction with protein three-dimensional structure calculation. Details are to learn from the following publications:

Herrmann, T., Güntert, P. & Wüthrich, K.

"Protein NMR structure determination with automated NOE-identification in the NOESY spectra using the new software ATNOS."

J. Biomol. NMR 2002 Nov; 24(3): 171-189.

Herrmann, T., Güntert, P. & Wüthrich, K.

"Protein NMR structure determination with automated NOE assignment using the new software CANDID and the torsion angle dynamics algorithm DYANA."

J. Mol. Biol. 2002 May; 319(1): 209-227.

Volk, J.; Herrmann, T.; Wüthrich, K.

"Automated sequence-specific protein NMR assignment using the memetic algorithm MATCH."

J. Biomol.NMR. 2008, 41, 127-138.

Fiorito, F.; Damberger, F.F.; Herrmann, T.; Wüthrich, K.

"Automated amino acid side-chain assignment of proteins using 13C- and 15N resolved 3D [1H, 1H]-NOESY." J. Biomol. NMR 2008, 42, 23-33.

This Software is composed of 3 types of files: executable (binary) files, configuration files and documentation files. Not included is the source code. (together "Software")

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Herrmann, T., Güntert, P. & Wüthrich, K.

"Protein NMR structure determination with automated NOE-identification in the NOESY spectra using the new software ATNOS."

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