Technology Offer

MARS – software for robust and automatic backbone assignment of protein NMR spectra

Ref.-No.: MI 0707-5990-MG

Background

MARS is a powerful program for robust automatic backbone assignment of proteins. MARS is applicable to proteins with extreme chemical shift degeneracy such as high molecular weight proteins and partially disordered or fully intrinsically disordered proteins. MARS is successfully used in many labs world-wide as evidenced by a huge number of citations.

Technology

Main features:

- MARS works with a wide variety of NMR experiments, from 3D triple-resonance experiments up to the most complex 6D and 7D APSY experiments.
- MARS is interfaced with CCPNmr Analysis enabling direct easy access to automatic assignment without export or re-import of data.
- MARS results can be directly read into the program SPARKY. Thus, several cycles of automatic assignment and manual validation can be performed.
- MARS allows to fix sequential connectivity, residue-specific as well as residue-type assignments.
- MARS enables the use of 3D structures, through the calculation of residual dipolar couplings and scalar couplings, for improved resonance assignment.
- MARS is applicable to both deuterated and protonated proteins.
- MARS offers unsurpassed accuracy for proteins with incomplete data.
- MARS has excellent tolerance against erroneous chemical shifts.
- MARS combines secondary structure prediction with statistical chemical shift distributions, which are corrected for neighboring residue effects.

Licensing Information

The MARS software is freely available for academic users. Industry and commercial users are invited to take a license. A non-exclusive right to use and display the software program is granted. Licensee will have the choice whether this shall be sent by e-mail or by regular mail (in the latter-case a CD- ROM is delivered).

Publication

1. Mars - robust automatic backbone assignment of proteins (2004) Young-Sang Jung and Markus Zweckstetter, J. Biomol. NMR, 30, 11-23.
2. Backbone assignment of proteins with known structure using residual dipolar couplings (2004) Young-Sang Jung and Markus Zweckstetter, J. Biomol. NMR, 30, 25-35.
3. Automatic assignment of the intrinsically disordered protein tau with 441-residues (2010) Narayanan RL, Dürr UH, Bibow S, Biernat J, Mandelkow E, Zweckstetter M, J. Am. Chem. Soc., 132, 11906-11907.

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