

RDC-ANALYTIC/RDC-PANDA License

January 21, 2010

RDC-ANALYTIC is a suite of programs for high-quality protein backbone fold determination from residual dipolar couplings (RDCs) (only two RDCs per residue are required) in one alignment medium, and a sparse set of nuclear Overhauser effect (NOE) data. RDC-PANDA (RDC-based SSE Packing with NOEs for Structure Determination and NOE Assignment), is a suite of programs for nuclear Overhauser effect (NOE) assignment and high-resolution structure determination starting with a global fold calculated from exact solutions to the residual dipolar coupling (RDC) equations. RDC-ANALYTIC and RDC-PANDA come as a single package, and both are developed in the lab of Prof. Bruce Donald at Duke University.

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You are required to cite our papers in any publications that use this code. The primary citation corresponding to this software is [1]. The papers that can be cited based-on or related-to this software are listed below.

- [1] Jianyang Zeng, Jeffrey Boyles, Chittaranjan Tripathy, Lincong Wang, Anthony Yan, Pei Zhou, and Bruce Randall Donald. High-resolution protein structure determination starting with a global fold calculated from exact solutions to the RDC equations. *Journal of Biomolecular NMR*, 45(3):265–281, 2009.
- [2] Bruce R. Donald and Jeffrey Martin. Automated NMR Assignment and Protein Structure Determination using Sparse Dipolar Coupling Constraints. *Progress in Nuclear Magnetic Resonance Spectroscopy*, 55(2):101–127, 2009.
- [3] Lincong Wang, Ramgopal R. Mettu, and Bruce R. Donald. A Polynomial-Time Algorithm for *De Novo* Protein Backbone Structure Determination from NMR Data. *Journal of Computational Biology*, 13(7):1276–1288, 2006.
- [4] Lincong Wang and Bruce Randall Donald. Analysis of a Systematic Search-Based Algorithm for Determining Protein Backbone Structure from a Minimal Number of Residual Dipolar Couplings. In *Proceedings of the 2004 IEEE Computational Systems Bioinformatics Conference (CSB’04)*, Stanford CA, pages 319–330, 2004.

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