Technology Offer

PALES software package

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NMR spectroscopy is a unique technique for the assignment of the constitution, configuration and conformation of small molecules, natural products, proteins, nucleic acid and oligosaccharides. NMR-derived residual dipolar couplings overcome limitations associated with traditional NMR data, avoid data misinterpretation and provide novel insights into structure-activity relationships. In order to leverage the full potential of residual dipolar couplings, however, powerful dedicated software and analysis tools are required.

Technology

Scientist from the Max-Planck-Institute for Multidisciplinary Sciences have developed the PALES (Prediction of ALignmEnt from Structure) software enabling effective and robust analysis of residual dipolar couplings. The key component of the PALES software is the prediction of the magnitude and orientation of the alignment tensor of a molecule weakly aligned in an anisotropic environment. PALES is highly flexible and works for small molecules, natural products, proteins, nucleic acid and oligosaccharides. PALES facilitates the reliable determination of the correct stereoisomer, enables unequivocal rapid determination of complex molecular structures from extremely sparse NMR data, provides insight into the quaternary structure of molecules, and enables refinement of conformational ensembles of small molecules, nucleic acids and proteins. In addition, efficient tools for the analysis of dipolar couplings are available.

Patent Information

A priority application for the P3D method was filed in January 2020.

Publication

Determination of Complex Small-Molecule Structures Using Molecular Alignment Simulation. Ibáñez de Opakua A, Klama F, Ndukwe IE, Martin GE, Williamson RT, Zweckstetter M.Angew Chem Int Ed Engl. 2020 Apr 6;59(15):6172-6176. doi: 10.1002/anie.202000311. Epub 2020 Feb 24.

https://mr.copernicus.org/preprints/mr-2020-32/mr-2020-32-manuscript-version3.pdf Extending the applicability of P3D for structure determination of small molecules Alain Ibáñez de Opakua and Markus Zweckstetter

NMR: prediction of molecular alignment from structure using the PALES software. Markus Zweckstetter Nature Protocols , Epub: 27 March, (2008) 679-690

Prediction of sterically induced alignment in a dilute liquid crystalline phase: aid to protein structure determination by NMR. Markus Zweckstetter and Ad Bax J. Am. Chem. Soc. ,122, (2000) 3791-3792

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