Enllaços sobre espectroscòpia de rmn

Cursos on-line

- e-MRI, Magnetic Resonance Imaging physics and technique course on the web.
- ENC - Experimental Nuclear Magnetic Resonance Conference contains PDF files of all Tutorial Lectures starting 2006.
- Chem 605 - Structure Determination Using Spectroscopic Methods. Instructor: Hans J. Reich, Department of Chemistry, University of Wisconsin, Madison.
- Advanced NMR A course on 2D NMR and the product operator formalism. Professor Gerd Gemmecker, 1999
- Basics of NMR Physics and Technique of NMR Spectroscopy. Joseph P. Hornak, Rochester Institute of Technology
- The Basics of MRI. Joseph P. Hornak, Rochester Institute of Technology

Wikibooks

- Basic Physics of Nuclear Medicine (Versió imprimible)

Llocs wiki

- NMR Wiki, is an open non-profit online NMR project (started on Nov 8th 2007). The goal of this site is to provide a collaborative informational resource to Spectroscopists, Chemists, Biologists and others using magnetic resonance techniques.
- SeRMN wiki, el **nostre** wiki 😎 per tot allò que afecta al funcionament del SeRMN.

Blogs on NMR

(Per ordre alfabètic del cognom de l'autor)

- Carlos Cobas' Blog, un dels autors inicials del programa Mestre-C (actualment Mnova) i fundador de la companyia Mestrelab Research SL. El blog està dedicat principalment al processament i interpretació dels espectres de rmn.
- Glen Facey's Blog, del servei de rmn de la Universitat d'Otawa. Tracta aspectes instrumentals, i com que tenen espectròmetres Bruker ens podem aprofitar.
- Solid-State NMR Literature Blog pel grup d'en Rob Schurko a la University of Windsor.
- Ryan's Blog on NMR Software, a ACD/Labs. Especialitzat en l'aplicació dels espectres de rmn a l'elucidació estructural i identificació dels components de mescles complexes.
- Stan's NMR Blog , tracta una mica de tot: la història de la rmn, les persones que la van protagonitzar, els fonaments químico-físics de la rmn, etcètera.

Calculadores on-line

Per RMN

- Calculators for NMR experiments: pulse length/power level, pulse length/field strength **(només per protó)**, coupling constant/delay time, NMR Temperature measurements.
- NMR and MRI related tools and short programs

Ús general

- UnitConversion.org is the ultimate resource for unit conversion. Use our free online unit converters to easily convert between different units of measurement. Simply select the appropriate unit converter from the lists below.

Basses de dades de desplaçaments químics

Solvents residuals

- The Solvent Chemical Shift Finder. The solvent chemical shift finder is an experimental database of over 100 different solvents and reagents which might appear in an NMR spectrum. For further details consult the references,
  - I. C. Jones, G. J. Sharman, J. Pidgeon. Spectral Assignments and Reference Data. 1-H and 13-C NMR data to aid the identification and quantification of residual solvents by NMR spectroscopy Magn. Reson. Chem., 2005, 43, 497-509.
  - H. E. Gottlieb, V. Kotlyar, A. Nudelman. NMR Chemical Shifts of Common Laboratory Solvents as Trace Impurities J. Org. Chem., 1997, 62, 7512-7515.

Compostos orgànics

- nmrshiftdb2 is a NMR database (web database) for organic structures and their nuclear magnetic resonance (nmr) spectra. It allows for spectrum prediction (13C, 1H and other nuclei) as well as for searching spectra, structures and other properties. Last not least, it features peer-reviewed submission of datasets by its users. The nmrshiftdb2 software is open source, the data is published under an open content license. Please consult the documentation for more detailed information. nmrshiftdb2 is the continuation of the NMRShiftDB project with additional data and bugfixes and changes in the software.
- Spectral Database for Organic Compounds (SDBS) is an integrated spectral database system for organic compounds,which includes 6 different types of spectra under a directory of the compounds. The six spectra are as follows, an electron impact Mass spectrum (EI-MS), a Fourier transform infrared spectrum (FT-IR), a 1H nuclear magnetic resonance (NMR) spectrum, a 13C NMR spectrum, a laser Raman spectrum, and an electron spin resonance (ESR) spectrum.
- Spektroskopische Tools/Spectroscopic Tools
- CSEARCH NMR Database
- NMR misinterpretation. Basic Misinterpretations, Typos and other Sad Events in NMR-Spectroscopy. **What is presented on this page?** This page holds examples of strange interpretation of NMR-data, either caused by missing basic knowledge about this method or

caused by typos or caused by any other reason. **What is intended with this page?** The sole intention of this page is to promote massive application of computer programs to verify structural and spectral data. In NMR-Spectroscopy we are in the lucky situation, that we have already algorithms available which allow us to check our analytical data in a(n) (semi-)automatic way. Routine application of these programs would increase the quality of the chemical literature in an easy and efficient manner.

- Automated Topology Builder (ATB) and Repository Version 2.2. The ATB and Repository is intended to facilitate the development of molecular force fields for Molecular Dynamics or Monte Carlo simulations of biomolecular systems. Applications include: the study of biomolecule:ligand complexes, free energy calculations, structure-based drug design, the refinement of x-ray crystal complexes. This site provides:
  - A repository for building blocks and interaction parameter files for molecules described using GROMOS force fields.
  - An automated builder to help generate building blocks for novel molecules, compatible with the GROMOS 54A7 force field and in formats appropriate for the GROMACS, GROMOS and LAMMPS simulation packages and CNS, Phenix, CCP4 and Refmac5 X-ray refinement packages.
  - A system topology file converter to generate AMBER topologies from GROMOS topologies.
  - Refined geometries for molecules within the repository.
  - Equilibrated starting coordinates for a range of biologically important systems.

Predicció de desplaçaments químics

nmrshiftdb

nmrshiftdb2 is a NMR database (web database) for organic structures and their nuclear magnetic resonance (nmr) spectra. It allows for spectrum prediction (13C, 1H and other nuclei) as well as for searching spectra, structures and other properties. Last not least, it features peer-reviewed submission of datasets by its users. The nmrshiftdb2 software is open source, the data is published under an open content license. Please consult the documentation for more detailed information. nmrshiftdb2 is the continuation of the NMRShiftDB project with additional data and bugfixes and changes in the software.

NMRdb

NMRdb is a web-based approach implementing a new java applet that enables to assign a chemical structure to the corresponding NMR spectrum by simply drawing lines between atoms and automatically characterized signals. Includes: NMR Simulator, NMR Resurrector, NMR Assigner and NMR Predictor.

There is a new HTML5 version of NMR Predictor that does not use the Java applet.

NMRPREDICT-Server

NMRPREDICT-Server. És un cul de sac sobre bases de dades i programes de predicció d'espectres de 13C. Per exemple,

- Spectral Similarity Search, entra els desplaçaments químics dels teus pics a l'espectre de 13C i et trobarà estructures amb espectres semblants.
- Aquest enllaç està estretament relacionat amb el programa comercial del mateix nom NMRPredict

ACD/Labs i-Lab

ACD/Labs i-Lab. Reduce the need for labor intensive experimental testing and literature searches, by using the online ACD/I-Lab prediction engine to predict physicochemical properties, NMR spectra and chemical shifts, and ADME toxicities. The browser-based I-Lab software also assesses prediction reliability and includes searchable content databases. I-Lab predictions are made using the same advanced algorithms that power our full desktop software suites, giving you the same highly accurate predictions without the need for individual software installations. A site license allows unlimited predictions for all of your organization's users, while the I-Lab for Intranets API can be implemented on servers behind your own firewalls. **How It Works:** Predictions are generated from structures, input in a variety of forms. Draw a structure in the I-Lab interface, paste a structure from ACD/ChemSketch, upload a SMILES string, or look up a compound in the built-in dictionary. Select a module to predict the property or spectra of interest, or generate a systematic name or structure for the molecule. Generate a report by saving the results to a PDF. **Available prediction modules:** Physicochemical Properties, ADME Properties, Toxicity Properties, NMR Spectra and Chemical Shifts Nomenclature. **I-Lab is also available for individual users as a credit-based system.**

Predicció de propietats químiques

- OSIRIS Property Explorer. The OSIRIS Property Explorer is an integral part of Actelion's inhouse substance registration system. It lets you draw chemical structures and calculates on-the-fly various drug-relevant properties whenever a structure is valid. Prediction results are valued and colour coded. Properties with high risks of undesired effects like mutagenicity or a poor intestinal absorption are shown in red. Whereas a green color indicates drug-conform behaviour.
- DataWarrior, an Open-Source Program for Data Visualization and Analysis with Chemical Intelligence. By openmolecules.org DataWarrior combines dynamic graphical views and interactive row filtering with chemical intelligence:
    - Scatter plots, box plots, bar charts and pie charts not only visualize numerical or category data, but also show trends of multiple scaffolds or compound substitution patterns.
    - Chemical descriptors encode various aspects of chemical structures, e.g. the chemical graph, chemical functionality from a synthetic chemist's point of view or 3-dimensional pharmacophore features. These allow for fundamentally different types of molecular similarity measures, which can be applied for many purposes including row filtering and the customization of graphical views.
    - DataWarrior supports the enumeration of combinatorial libraries as the creation of evolutionary libraries. Compounds can be clustered and diverse subsets can be picked.
    - Calculated compound similarities can be used for multidimensional scaling methods, e.g. Kohonen nets.
    - Physicochemical properties can be calculated, structure activity relationship tables can be created and activity cliffs be visualized.

Metabolòmica

- NMR Search @ the Human Metabolome Database
- BioMagResBank - Metabolomics Standard Compounds
- Metabolite NMR Search a la Human Metabolome Database
- Interactive Metabolic Pathways Map at Sigma-Aldrich.
- Generic Model Organism Database project, a collection of open source software tools for managing, visualising, storing, and disseminating genetic and genomic data.

BioCyc

The BioCyc collection of Pathway/Genome Databases (PGDBs) provides an electronic reference source on the genomes and metabolic pathways of sequenced organisms. BioCyc PGDBs are generated by software that predicts the metabolic pathway complements of completely sequenced organisms from their genome sequences. Furthermore, BioCyc PGDBs include the results of a number of other computational inference procedures applied to these genomes, including predictions of which genes code for missing enzymes in metabolic pathways, and predicted operons. The BioCyc website provides a suite of software tools for database searching and visualization, for omics data analysis, and for comparative genomics and comparative pathway questions.

BioCyc contains 2988 databases as of June 11th (version 17.1). The most comprehensive databases are part of *Tier 1 Databases* and they are required to have received at least one year of literature-based curation by scientists. Currently they are:

- EcoCyc Escherichia coli K-12 substr.MG1655. SRI International.
- MetaCyc Metabolic pathways and enzymes from over 2063 organisms. SRI International.
- HumanCyc 250 metabolic pathways. SRI International.
- AraCyc Arabidopsis thaliana S. Rhee, Department of Plant Biology, Carnegie Institution, USA.
- YeastCyc Saccharomyces cerevisiae. SGD Curators, Stanford U., USA.
- LeishCyc Leishmania major. Friedlin Bio21 Molecular Science and Biotechnology Institute, University of Melbourne, Australia.

Find below a more detailed description of the most relevant databases for biomedical studies.

- MetaCyc is a database of non-redundant, experimentally elucidated metabolic pathways. MetaCyc contains more than 2097 pathways from more than 2460 different organisms [more], and is curated from the scientific experimental literature. MetaCyc contains pathways involved in both primary [def] and secondary [def] metabolism, as well as associated compounds, enzymes, and genes.
- HumanCyc is a bioinformatics database that describes human metabolic pathways and the human genome. By presenting metabolic pathways as an organizing framework for the human genome, HumanCyc provides the user with an extended dimension for functional analysis of *Homo sapiens* at the genomic level. For example, HumanCyc has tools for analysis of human metabolomics and gene-expression data.
- MouseCyc is a database of curated biochemical pathways data for the laboratory mouse that can be integrated with functional and phenotypic data from MGI.

ExPASy

ExPASy is the SIB Bioinformatics Resource Portal which provides access to scientific databases and software tools (i.e., resources) in different areas of life sciences including proteomics, genomics, phylogeny, systems biology, population genetics, transcriptomics etc. (see Categories in the left menu). On this portal you find resources from many different SIB groups as well as external institutions.

MetaboHunter

MetaboHunter is a web server application for semi-automatic assignment of 1D NMR spectra of metabolites. MetaboHunter provides tools for metabolite identification based on spectra or peak lists with three different search methods and with possibility for peak drift in a user defined spectral range. The assignment is performed by comparison with two major publically available databases (HMDB, MMCD) of NMR metabolite standard measurements. In this work we present the Web tool with detailed testing of the methods provided in the Supplementary data.

- MetaboHunter: an automatic approach for identification of metabolites from 1H-NMR spectra of complex mixtures. Dan Tulpan et al., BMC Bioinformatics 2011, 12:400 PDF Supplementary data

Taules de desplaçaments químics

- Proton chemical shifts
- Carbon chemical shifts

Taules periòdiques

- WebElements NMR Periodic Table
- Enhanced NMR Periodic Table at Texas A&M University.
- NMR Periodic Table at Rider University.
- NMR Periodic Table at Hebrew University.

Fonaments de la rmn

- Espectroscòpia de rmn a la Wikipedia.
  - Corrent d'anell aromàtic
  - Desplaçament químic
  - Susceptibilitat magnètica
- Notes dels cursos impartits pel Dr. Oliver Zerbe de l'ETH Zurich.
  - Lecture Course: NMR Spectroscopy. (fitxer PDF, 142 pàgines)
  - Practical NMR course (March 2006). Disponible també en format per imprimir , on s'ha eliminat el fons de les diapositives. (fitxers PDF, 111 diapositives)
  - Script for the "NMR / Protein Structure" course. (fitxer PDF, 27 pàgines)
  - Slides for the structure/dynamics/folding course section. (fitxer PDF, 165 diapositives)
- Notes dels cursos impartits pel Dr. Arthur S. Edison, Associate Professor, University of Florida
  - Molecular Structure and Dynamics by NMR Spectroscopy (BCH 6745 and BCH 6745L)

Programari d'interés

- NMRbox is a resource for biomolecular NMR (Nuclear Magnetic Resonance) software. It provides tools for finding the software you need, documentation and tutorials for getting the most out of the software, and cloud-based virtual machines for executing the software.
- rNMR is an open source software package for visualizing and interpreting one and two dimensional NMR data. In contrast to most existing 2D NMR software, rNMR is specifically designed for high-throughput assignment and quantification of small molecules. As a result, rNMR supports extensive batch manipulation of plotting parameters and has numerous tools for expediting repetitive resonance assignment and quantification tasks.
- SPINUS (Structure-based Predictions In NUclear magnetic resonance Spectroscopy) is an on-going project for the development of structure-based tools for fast prediction of NMR spectra. SPINUS - WEB currently accepts molecular structures via a Java molecular editor, and estimates 1H NMR chemical shifts and coupling constants. The predictions are obtained from ensembles of previously trained feed-forward neural networks, and corrected with data from an additional memory.
- PLT for Windows. PLT is a program for drawing chemical structures and creating hard copy on printers and other Windows-supported output devices.
- AcornNMR Periodic Table. This is an Excel spreadsheet which calculates resonant frequencies for all magnetically active nuclei. Just enter your proton frequency (in cell B5) and all others are calculated from it.

Altres llocs web d'interés

- Print Free Graph Paper. Save yourself money and a trip to the store! Print graph paper free from your computer. All graph paper files are optimized PDF documents requiring Adobe Reader for viewing. Available formats: Cartesian, Engineering, Polar, Isometric, Logarithmic, Hexagonal, Probability, and Smith; in Letter or Din a4 paper size; in inches or millimeters measuring units, and several chart spacing.
- Martindales Center conté un munt d'enllaços d'interès per RMN i MRI, però no he tingut temps de comprovar la seva vàlua i utilitat.
- Organic Chemistry Portal. The Organic Chemistry Portal offers an overview of recent topics, interesting reactions, and information on important chemicals for organic chemists.
- eMolecules empowers researchers to explore uncharted chemical and biological space and deliver more efficient drug discovery programs. Our promise to drug discovery researchers is that we will aim to facilitate:
    - **exploration** of unchartered chemical and biological space with our database of over 8 million compounds available from our global network of trusted suppliers.
    - **evaluation** of the best source of molecules for their projects based upon suppliers' availability, delivery time and pricing data which we normalize, update and curate monthly.
    - **expedition** of their drug discovery programs by reducing the barriers, time and costs associated to acquiring molecules.
- El portal de la Division of Organic Chemistry, American Chemical Society inclou uns apartats sobre RMN que procedeixen en gran part de la “Prof. Hans Reich's collection of various topics on NMR. Most of this content originated from his Chem 605 Course at the University of Wisconsin - Madison.”.
    - General NMR
    - NMR Data

- Multinuclear NMR Data