Annotated Bibliography NMR – Charles Holcombe

1. Mlynarik, Vladimir. (2016). Introduction to nuclear magnetic resonance. Analytical Biochemistry. 529. 10.1016/j.ab.2016.05.006.
	1. Very basic introduction article that uses classic physics to describe magnetic resonance. It covers basic physics, nuclear relaxation, chemical shifts, spin coupling, and spectral line intensity. The discussion is then briefly extended to MRI. The first few slides of my presentation came from this publication.
2. Hong, Mei et al. “Membrane protein structure and dynamics from NMR spectroscopy.” Annual review of physical chemistry 63 (2012): 1-24.
	1. In depth review paper that touches on magic angle spinning and sample oriented solid-state NMR, and then reviews the latest material and methods related to potassium, proton, GPCRs, β-sheet-rich proteins, viral fusion proteins, and phospholamban membrane proteins. You will need to investigate the references to get any in depth information from this review paper, but it gives you a great starting point to investigate a number of different current topics.
3. Ortega-Roldan, Jose Luis et al. “Solution NMR studies reveal the location of the second transmembrane domain of the human sigma-1 receptor” FEBS letters vol. 589,5 (2015): 659-65.
	1. Authors did solution NMR studies on a novel S1R construct (removed first 35 residues) to study the second transmembrane. They utilized a TROSY NMR to acquire data and verified with circular dichroism spectrum. Then they discuss the methods of analyzing the data with included chemical shift-based secondary structure analysis, 13Cα chemical shift index, 1H–15N heteronuclear NOEs, relaxation ratios and chemical shift perturbations. They present the characterized secondary structure of S1R missing only 8 residues N-terminus and the first transmembrane domain. The second transmembrane helix, TM2, was found to be composed of residues 91–107.
4. Opella, Stanley J. “Solid-state NMR and membrane proteins” *Journal of magnetic resonance (San Diego, Calif. : 1997)* vol. 253 (2014): 129-37.
	1. A more in-depth review of solid state NMR. The introduce different coupling issues and how they are resolved or minimized. They also discuss the three basic approaches to obtaining high resolution (motional averaging, spin dilution, and spin manipulation) and the different techniques to help do so (MAS, oriented sample, and rotationally aligned SS NMR)
5. High-resolution NMR studies of antibiotics in cellular membranes Medeiros-Silva J., Jekhmane S., Paioni A.L., Gawarecka K., Baldus M., Swiezewska E., Breukink E., Weingarth M. (2018) Nature Communications, 9 (1) , art. no. 3963
	1. High level paper that investigates alternative antibiotic pathways to combat common antibiotic resistance. They investigate Lipid II, a promising new therapeutic target. Little is known about it now due to the difficulty studying small molecule drug receptors in cell membranes. They used very sensitive ssNMR techniques (Dynamic Nuclear Polarization – increases response of NMR by ratio of electron/proton gyromatic ratio in simplest form) to show this is a viable antibiotic alternative. A robust knowledge of both biology and NMR is needed to get through this one.
6. Bajaj VS, Mak-Jurkauskas ML, Belenky M, Herzfeld J, Griffin RG (2009) Functional and shunt states of bacteriorhodopsin resolved by 250 GHz dynamic nuclear polarization-enhanced solid-state NMR. Proc Natl Acad Sci USA **106**:9244–9249.
	1. Authors discuss the theoretical advantages of using dynamic nuclear polarization NMR. They specifically discuss the advantages when used to acquire data on bacteriorhodopsin, a bacteria protein that transports protons across cytoplasmic membrane. The use of DNP resulted in a 90-fold sensitivity increase in one dimension. Thus, to acquire a 2D NMR, the technique reduced the acquisition time by a factor of 8,100. They go on to discuss the protein in detail that can only be achieved with DNP.
7. John L. Markley, William Milo Westler, Biomolecular NMR: Past and future, Archives of Biochemistry and Biophysics, Volume 628, 2017, Pages 3-16, ISSN 0003-9861, <https://doi.org/10.1016/j.abb.2017.05.003>.
	1. An easy and interesting read from in which the authors discuss the evolution of NMR from the 1970’s to present as it relates to their labs (Carnegie-Mellon University, Purdue, University of Wisconsin-Madison). They touch on instrumentation (hardware and software), sample preparation, and pulse sequences among other things.
8. Qin H, Miao Y, Cross TA, Fu R. Beyond Structural Biology to Functional Biology: Solid-State NMR Experiments and Strategies for Understanding the M2 Proton Channel Conductance. The Journal of Physical Chemistry B. 2017;121:4799–4809. doi: 10.1021/acs.jpcb.7b02468
	1. The authors investigate the full length M2 in protein (M2FL) from the Infleunza A Virus. They describe the various SSNMR methods used to obtain the kinetics of and dynamics of the proton channel. These data from numerous spectra are illustrated to describe the structure function relationship. This paper is difficult to follow without a working knowledge of SSNMR.
9. Opella, S. J., & Marassi, F. M. (2017). Applications of NMR to membrane proteins. *Archives of biochemistry and biophysics*, *628*, 92-101. doi: 10.1016/j.abb.2017.05.011
	1. Phenomenal review of pros and cons of NMR and this paper also highlights the differences in capabilities of solution versus solid-state. The advancements of solution based NMR include discussions of specialized detergent-free lipid bilayer nanodiscs (as these represent the native environment of membrane proteins better than detergents). The discussion extends to oriented sample and magic angle spinning solid state NMR, but not as in-depth as the previous article. This paper is relatively easy to read and gives a great overview of the topic.
10. Concepts and Methods of Solid-State NMR Spectroscopy Applied to Biomembranes Trivikram R. Molugu, Soohyun Lee, and Michael F. Brown Chemical Reviews 2017 117 (19), 12087-12132 DOI: 10.1021/acs.chemrev.6b00619
	1. Very in-depth and math heavy review of advanced SSNMR techniques. The section I found most interested was the explanation of deuterium and quad coupling as it applies to NMR. Early literature required half spin/odd number protons for NMR, but advanced techniques allow deuterium (spin = 1) NMR and direct measurement of quadrupolar coupling.

Websites

1. <https://nationalmaglab.org/user-facilities/nmr-mri/nmr-mri-resources>
	1. The National High Magnetic Field Laboratory is a huge resource right down the road! Plus they have a website with a lot of information.
2. <https://chem.libretexts.org/>
	1. Open access, multi-institute website covering a lot of science. You can take entire courses through various universities, or search for specific material like the NMR article below: [https://chem.libretexts.org/Textbook\_Maps/Physical\_and\_Theoretical\_Chemistry\_Textbook\_Maps/Supplemental\_Modules\_(Physical\_and\_Theoretical\_Chemistry)/Spectroscopy/Magnetic\_Resonance\_Spectroscopies/Nuclear\_Magnetic\_Resonance/Nuclear\_Magnetic\_Resonance\_II](https://chem.libretexts.org/Textbook_Maps/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_%28Physical_and_Theoretical_Chemistry%29/Spectroscopy/Magnetic_Resonance_Spectroscopies/Nuclear_Magnetic_Resonance/Nuclear_Magnetic_Resonance_II)
3. <https://www.khanacademy.org/science/organic-chemistry/spectroscopy-jay/proton-nmr/v/introduction-to-proton-nmr>
	1. Khan Academy videos offer an easy to understand introduction into concepts and is usually a great starting point for a new topic.
4. <http://www.cis.rit.edu/htbooks/nmr/nmr-main.htm>
	1. Online book that covers the basics of NMR
5. <http://demonstrations.wolfram.com/NMRSignalProcessingLabTwoSpins12/>
	1. An online signal processing application to better understand fourier transforms and NMR
6. <http://www.chemspider.com/>
	1. Compound resource that even has NMR spectra available for download
7. <https://link.springer.com/journal/723>
	1. Applied Magnetic Spectroscopy journal – great resource for articles
8. <https://www.youtube.com/user/ANZMAG/videos>
	1. This video series includes 14 James Keeler lectures that cover his book, Understanding of NMR Spectroscopy.
9. <https://link.springer.com/journal/10858>
	1. Journal of Biomolecule NMR
10. <http://nmrwiki.org/wiki/index.php?title=Main_Page>
	1. NMR Wiki – exactly what it sounds like. The site is dated, but has valuable education material nonetheless.