

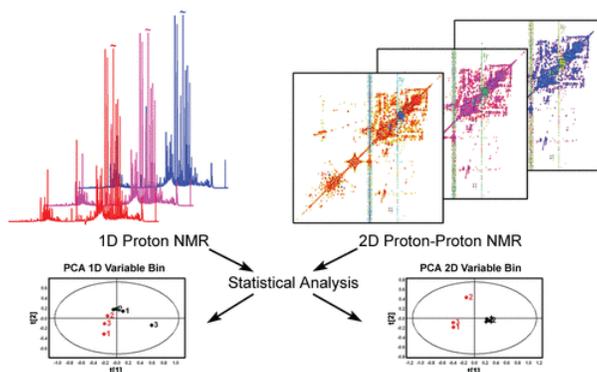
7.5: Uses for 2-D NMR Spectroscopy

Learning Objectives

- Learn in what instances scientists use 2-D NMR
- Understand practical applications of 2-D NMR

It has been previously mentioned in this chapter that the major advantage for using 2-D NMR over 1-D NMR is the ability to distinguish between overlapping signals that exist in larger molecules. 2-D NMR is incredibly important in biological and polymer chemistry to elucidate the three-dimensional structure of these large macromolecules. In these cases, HSQC can be used to determine the profile of metabolites in low concentrations (microMolar) accurately. TOCSY has been utilized to show changes in tumor cells and identify biomarkers associated with these cells. Molecular dynamics can be studied using 2-D NMR spectroscopy to map the molecule's internal mobility patterns. With molecular dynamics the loose ends of proteins can be studied and elucidated to learn more about the flexible surface areas often lost in other methods. 2D NMR has many more applications beyond protein NMR, including characterization of pharmaceuticals, temperature dependence of carbohydrate conformations, and metabolomics, to just name a few.

2-D NMR is often used in metabolic profiling like in the example below. This is due to the fact that NMR is not a destructive analysis, quantitative, reproducible and gives a lot of information about the sample.



Using TOCSY, this particular study compared the global metabolic profiles of urine obtained from two types of mice, specifically of wild-type and a knockout. Both 1-D and 2-D NMR experiments were run to determine if statistical differences between the techniques, especially when looking at low abundance metabolites. Both 1-D and 2-D NMR data could differentiate between the two types of mice, but only the 2-D data could be used to show statistically relevant changes in the low abundance metabolites. The con of 2-D NMR data is that it takes longer to obtain the data compared to 1-D NMR data collection, however, the data obtained resulted in a more meaningful and comprehensive metabolic profile, aided in metabolite identifications, and minimized ambiguities in peak assignments.² This is just one example of how 2-D NMR has been applied.

References

1. <https://www.news-medical.net/life-sc...lications.aspx>; Accessed July 29, 2022.
2. *J. Proteome Res.* 2008, 7, 2, 630–639 Publication Date: December 15, 2007 <https://doi.org/10.1021/pr700594s>

7.5: Uses for 2-D NMR Spectroscopy is shared under a [not declared](#) license and was authored, remixed, and/or curated by Lauren Reutenauer.