# Analysis of Contaminated Environments by Diffusion Ordered Spectroscopy (DOSY) and ACD/ChemAnalytical Workbook

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## Introduction

Groundwater is a vital part of our modern society, supplying a significant amount of the water we use in our homes, agricultural fields, and industries every day. Given its importance, we are all affected by the environmental, health, and economic consequences when groundwater is polluted with hazardous chemical contaminants. Characterizing the nature and extent of contamination present at a site is a key step when developing risk assessments and implementing remedial solutions for contaminated groundwater. This information allows us to have a clearer understanding of what exactly is present, how it may have gotten there and how it is responding to remedial activities. Conventional analytical approaches are usually designed for the targeted analysis of a suite of suspected contaminants. These methods, however, often fail to identify compounds that are not normally analyzed for, including degradation products, proprietary chemicals, and other species for which standards are not readily available. NMR spectroscopy provides a unique analytical approach to present a more complete, and unbiased understanding of the nature and extent of organic compounds present at contaminated sites undergoing assessment and monitoring activities.

## Discussion

Groundwater samples were taken from an industrial site currently undergoing remediation. The extent of contamination at this site was such that the contaminants formed their own free flowing non-aqueous phase that sits beneath the water table. A few drops of this sample were dissolved in DMSO and analyzed using high resolution NMR methods, including Diffusion-Ordered Spectroscopy (DOSY). The $^{1}$H NMR spectrum of this sample, as shown in Figure 1, is complex with many overlapping signals. This sample contains numerous aromatic and aliphatic compounds, as expected based on the history of the site.

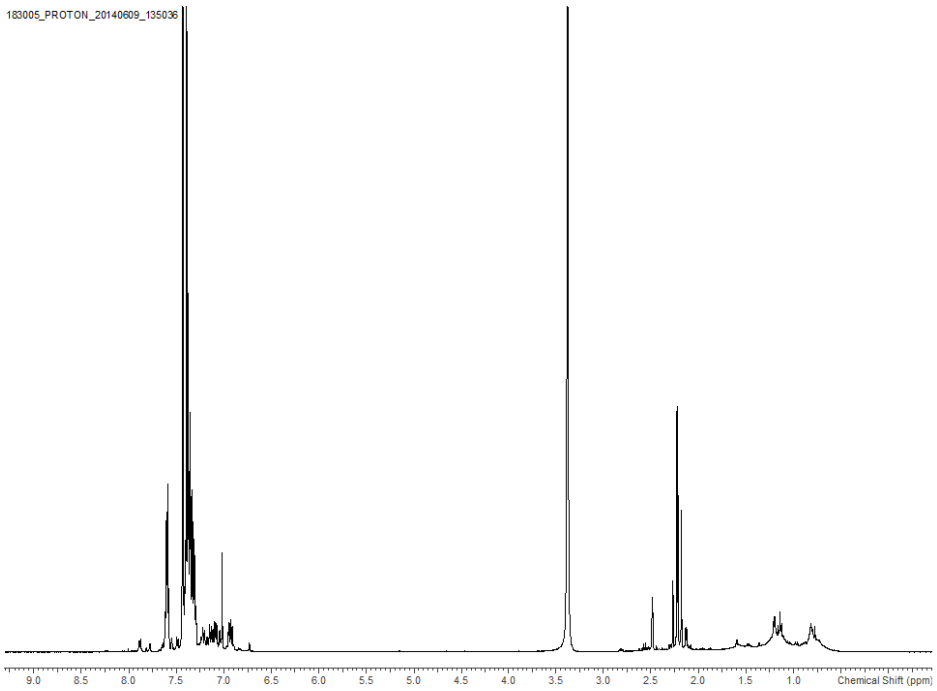


***Figure 1**: A sample $^{1}$H NMR spectrum of a sample taken from a contaminated site.*

$^{1}$H DOSY NMR data was acquired for this sample in an effort to deconvolute the complex spectrum. The DOSY tool with ACD/ChemAnalytical Workbook is a simple, reliable tool that was used to align, phase, and base line correct the raw DOSY data, as shown in Figure 2. The region around the DMSO-$H_2O$ signal was set as a dark region (to be ignored by the software when generating the DOSY plot). Automated peak fitting (Gauss+Lorentz) across the entire series was used to assist in deconvolution of each spectrum prior the calculation of the DOSY spectrum.

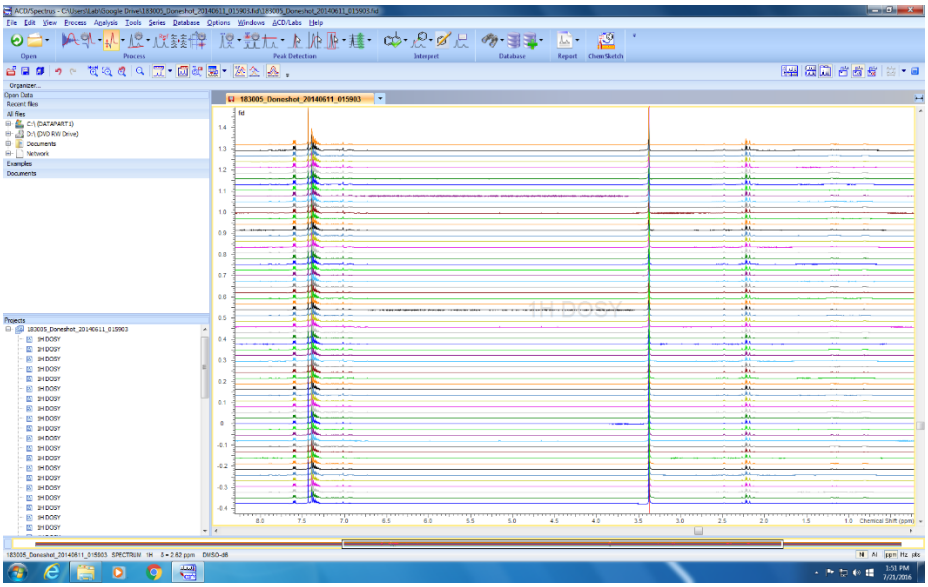

***Figure 2**: A sample screen capture of the Gradient Series of $^{1}$H NMR spectra prior to DOSY calculation.*

The DOSY NMR spectrum of this sample provides improved clarity in the complex $^{1}H$ spectrum of this sample. This information was useful in identifying dozen of compounds present at this site based on both chemical structure and relative size, including chlorinated aromatics, methyl aromatics, and aliphatic hydrocarbons.

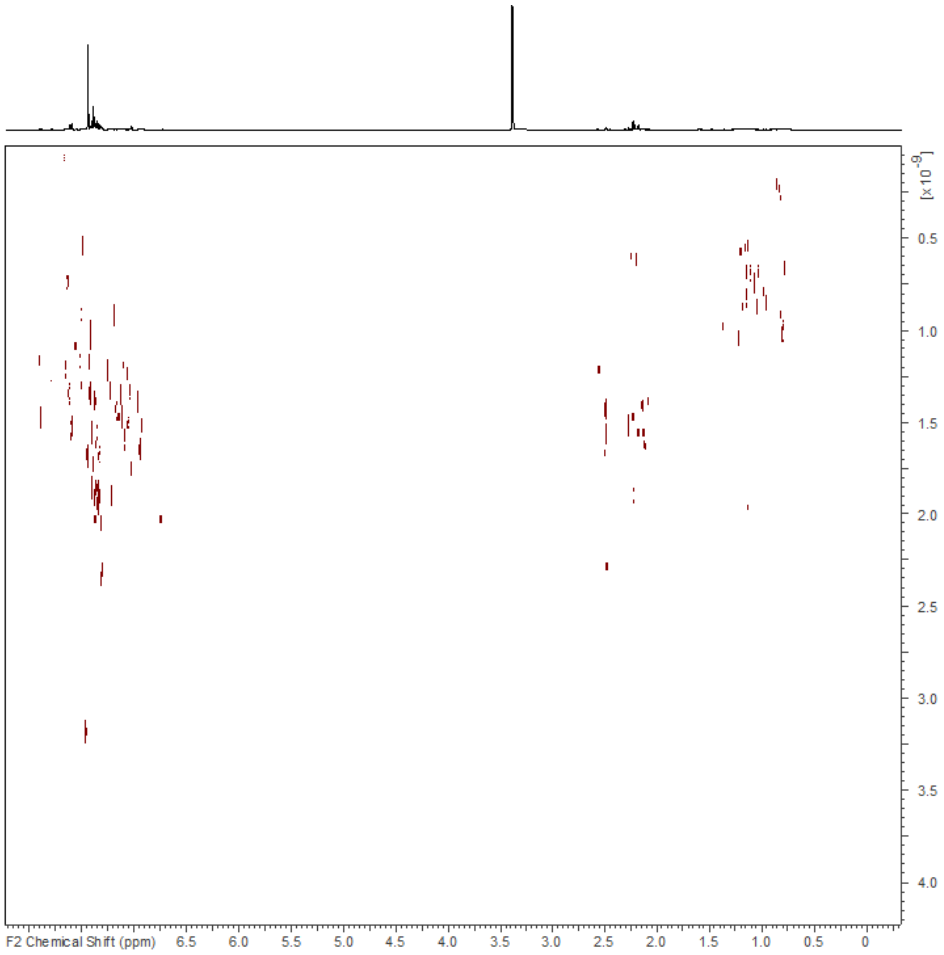


***Figure 3**: The peak-fitted $^{1}H$ NMR DOSY spectrum where the $^{1}H$ resonances are dispersed along the second dimension (diffusion coefficient). The separation along the second dimension allows for several slices to be extracted at a particular diffusion coefficient which represents either a single compound and/or a smaller group of compounds of similar size.*

## Conclusion

DOSY NMR is able to provide the deconvolution necessary to identify many compounds in a complex $^{1}H$ NMR spectrum of a sample taken from a contaminated site. The ability to apply peak fitting prior to generation of the DOSY spectrum increases the resolution along the diffusion dimension, decreasing contour overlap, and allowing for easy component extraction and identification from a complex mixture.