

# Pure shift NMR: overview, applications and tips and tricks

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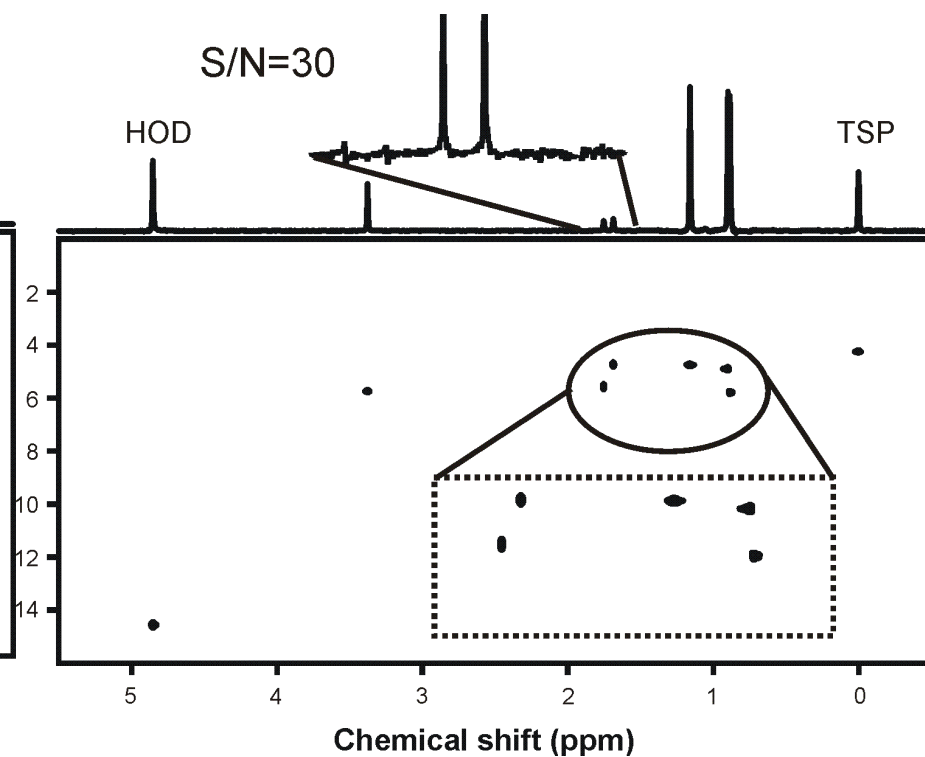
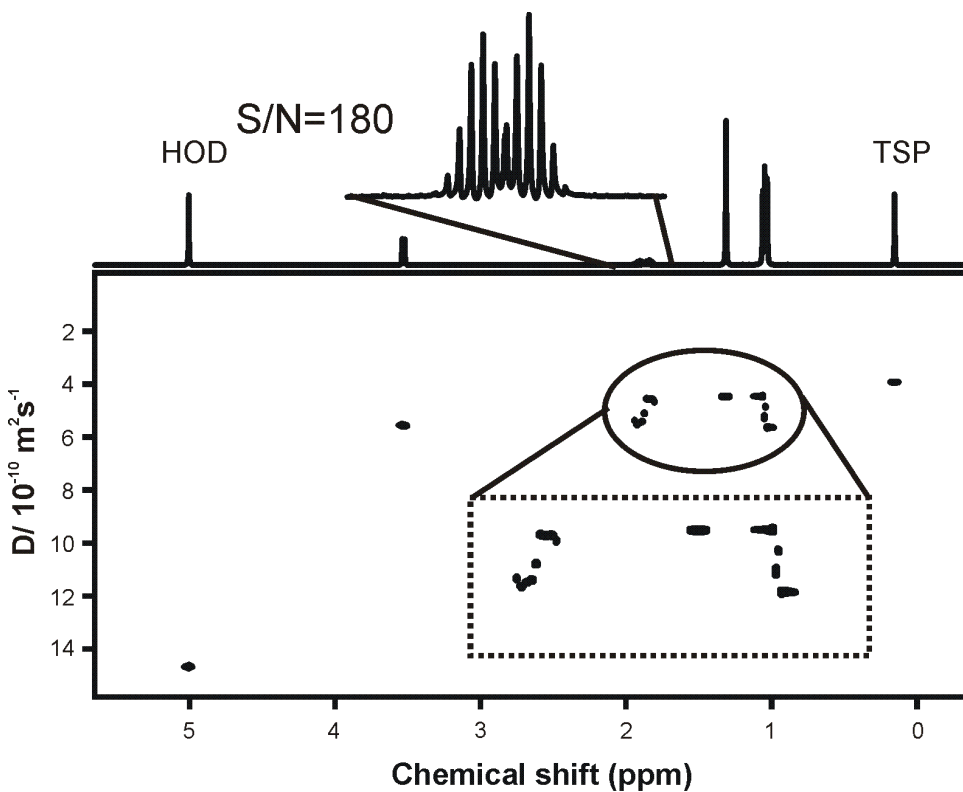
**NMR Methodology Group**  
University of Manchester

IVAN online workshop.  
June 14<sup>th</sup>, 2021

# Manchester pure shift: a humble start

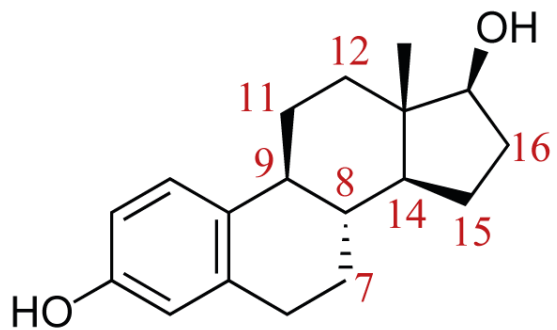
conventional DOSY

pure shift DOSY

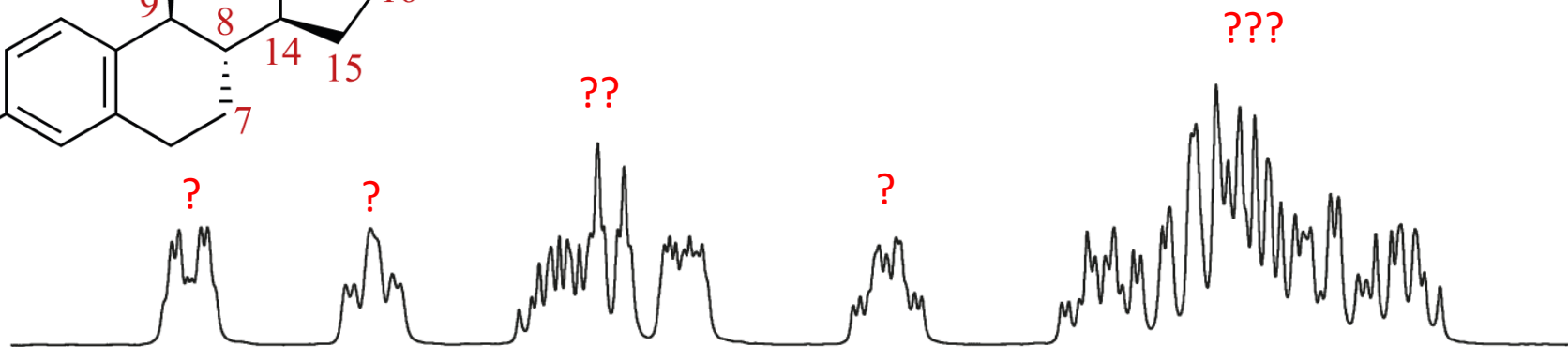


400 MHz DOSY spectra of 2-methyl-1-propanol and 2,3-dimethyl-2-butanol

# Simplifying spectra

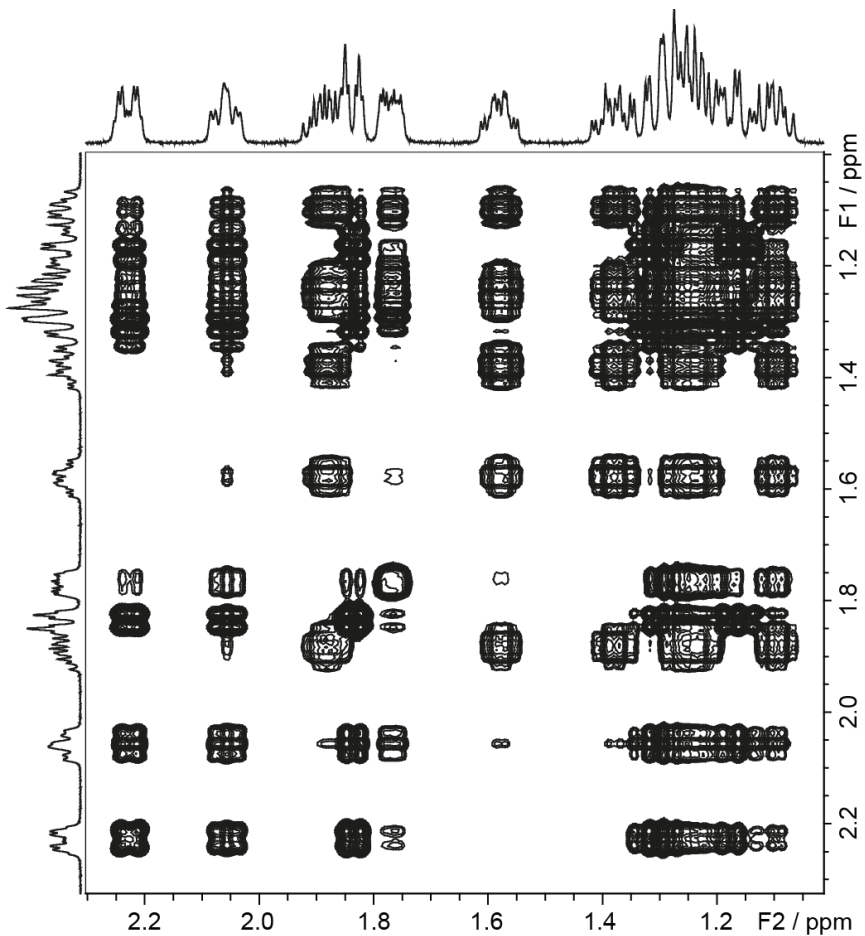


Estradiol: 500 MHz  $^1\text{H}$  spectrum



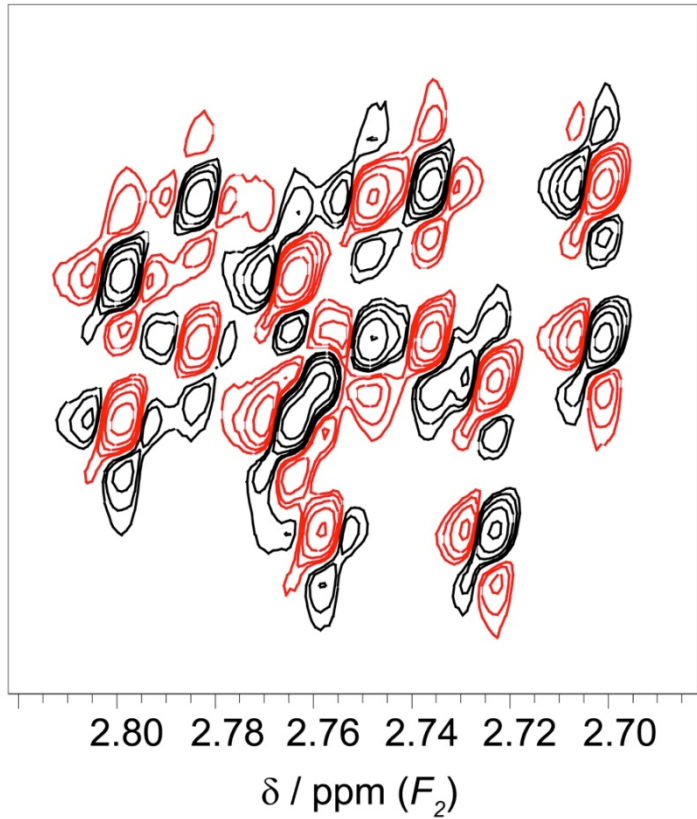
# Simplifying spectra, and retaining coupling information

## Estradiol: 500 MHz TOCSY



# pure shift 3QF- COSY cross peaks

a) Fully  $^1\text{H}$ - $^1\text{H}$  coupled



# Speakers

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## Introduction

**Teodore Parella**

Universitat Autònoma de Barcelona

## Tips and tricks

**Ralph Adams**

University of Manchester

## Applications

**Christina Thiele**

Technische Universität Darmstadt