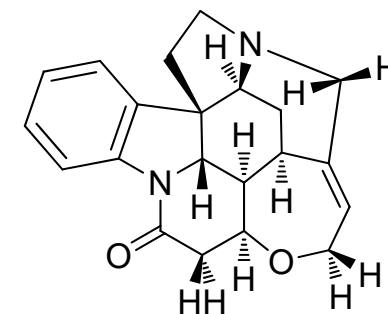
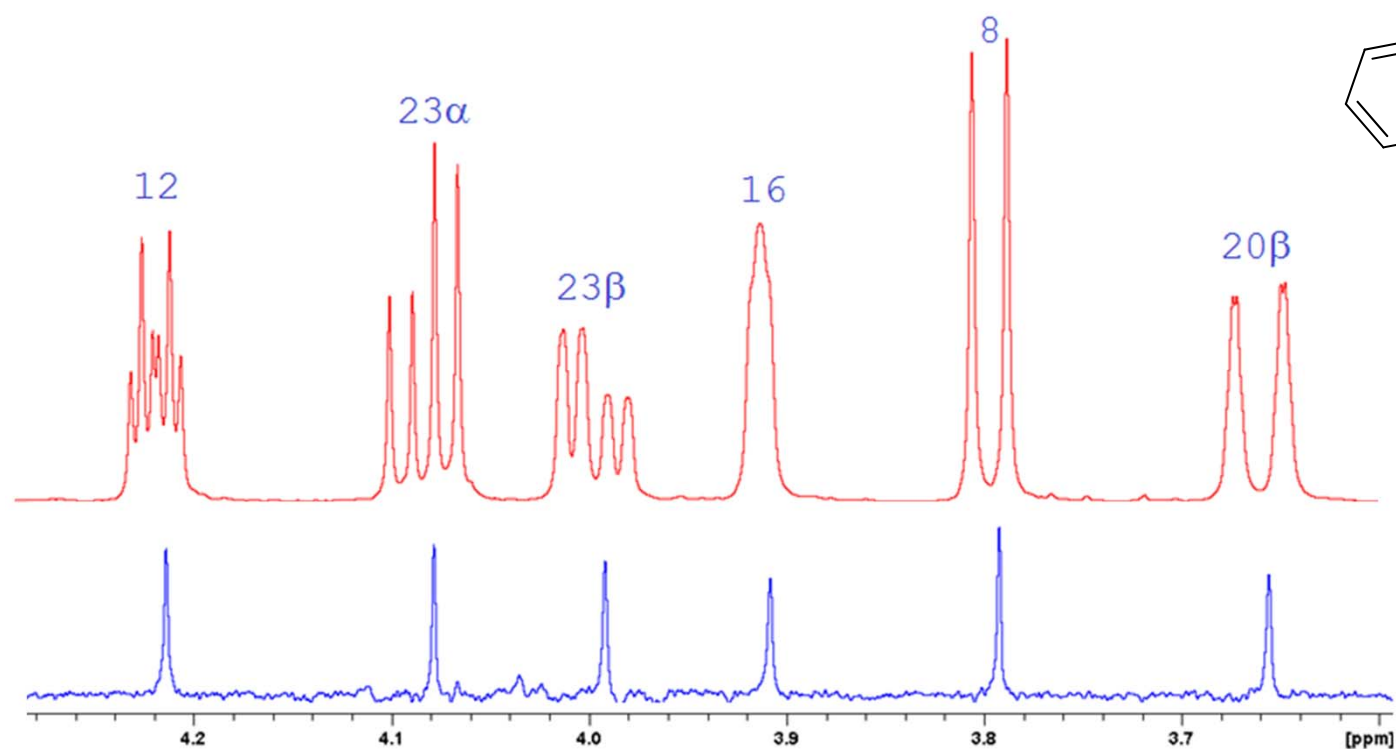


IVAN Pure Shift Workshop



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Part III Applications

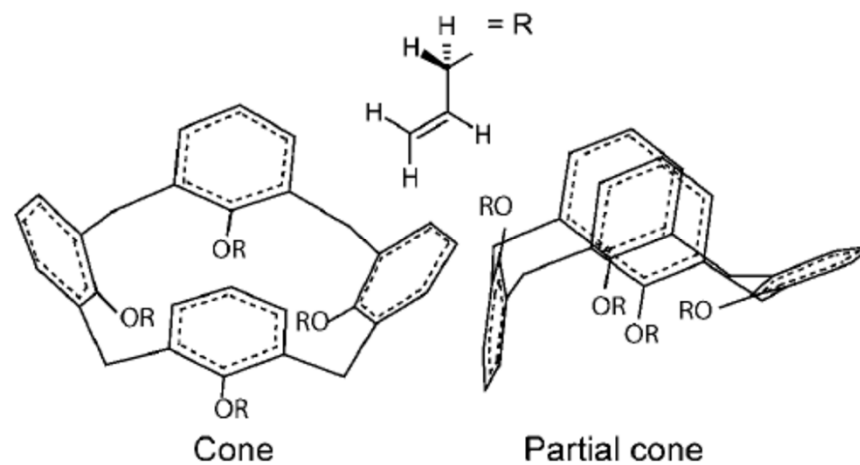
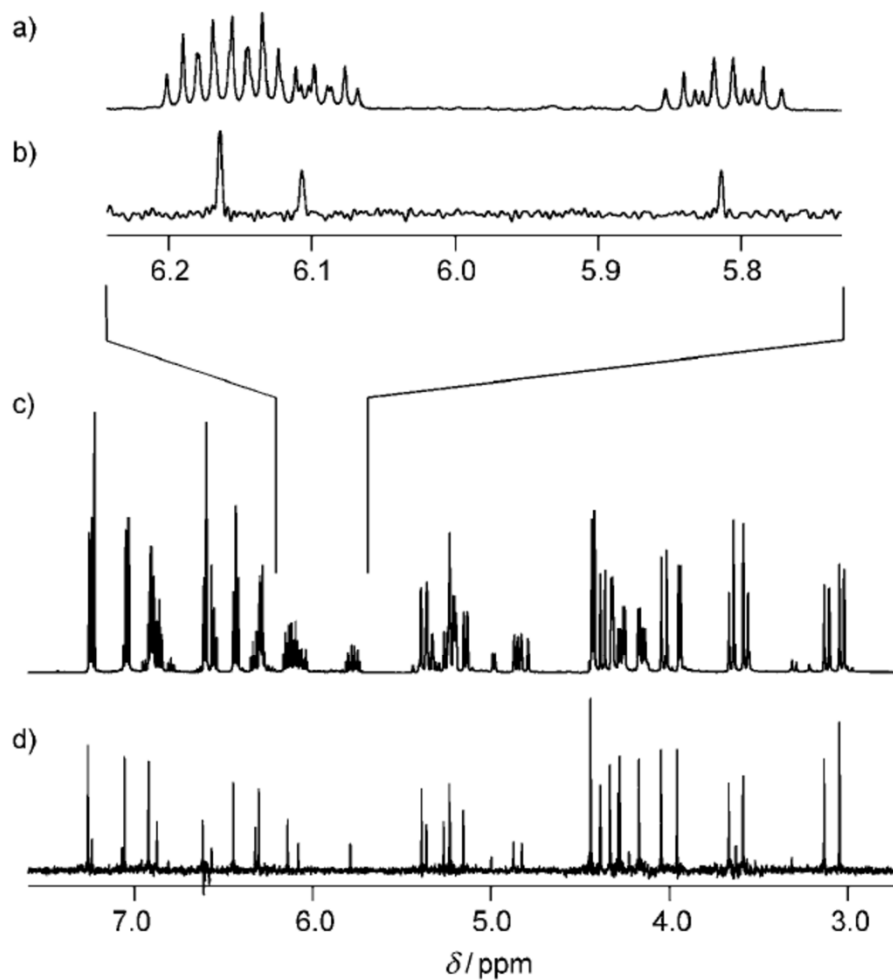


Main Reasons for overlapping signals



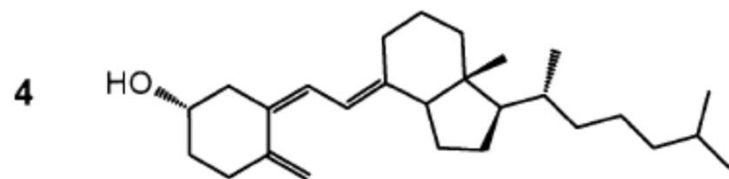
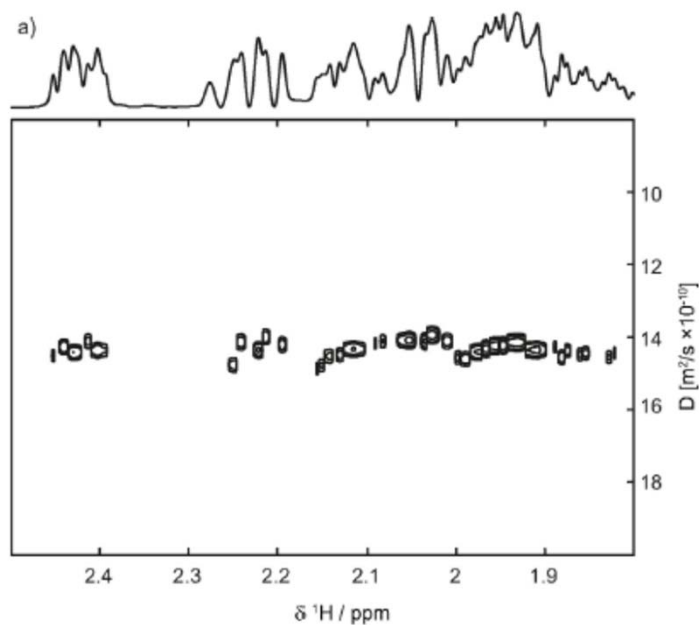
-
- Mixtures of compounds
 - Overlapping multiplets in complex compounds

Mixtures

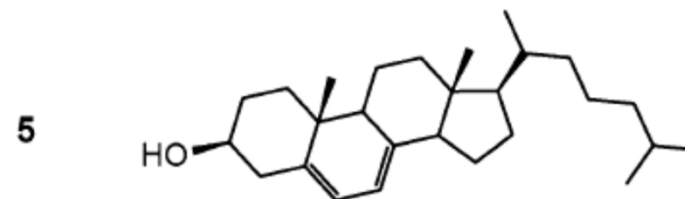
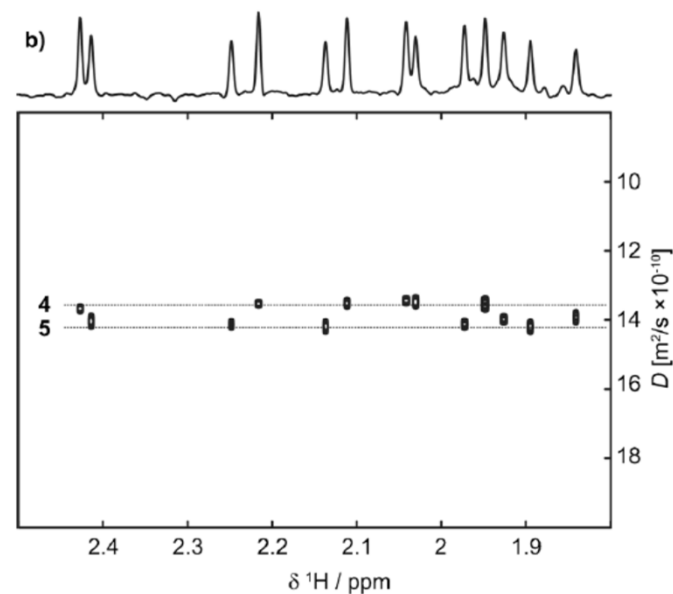


Mixtures: Resolution of Provititamin D₃ vs. Vitamin D₃ via DOSY

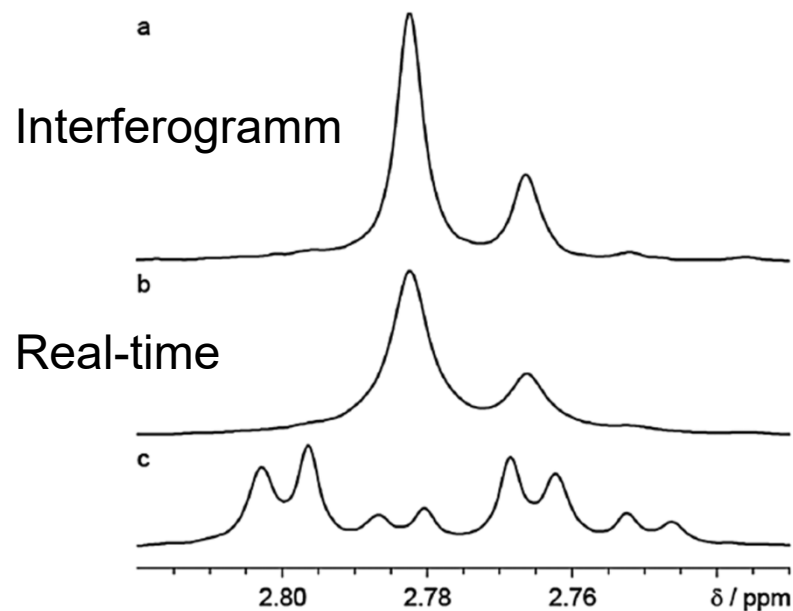
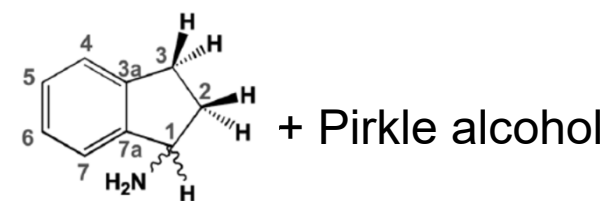
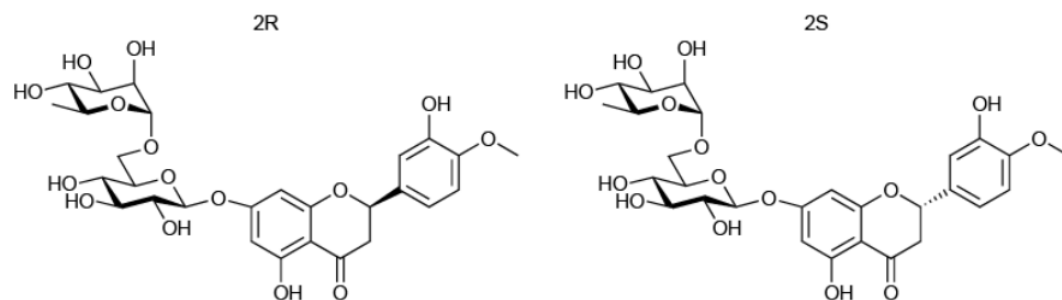
Oneshot DOSY



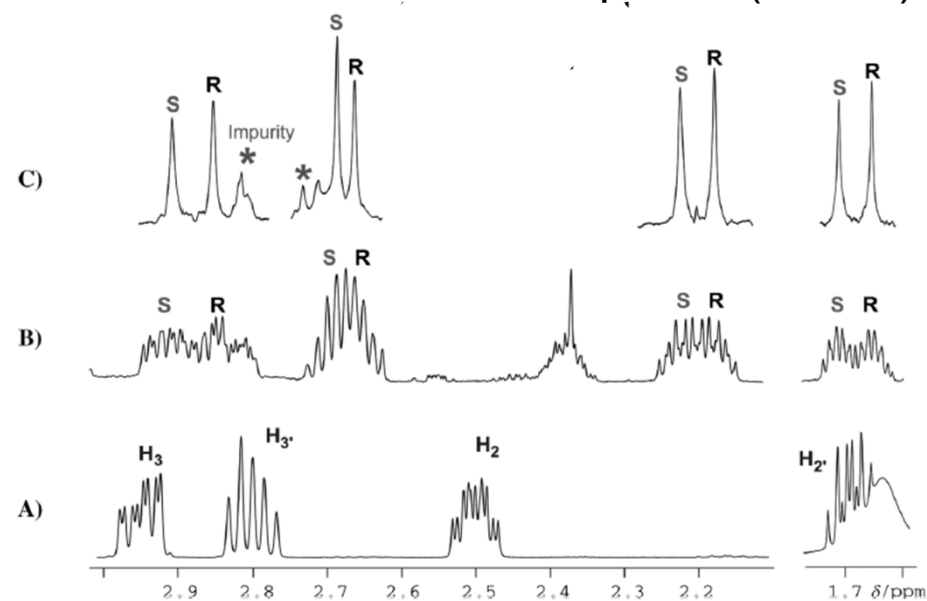
PSYCHE iDOSY



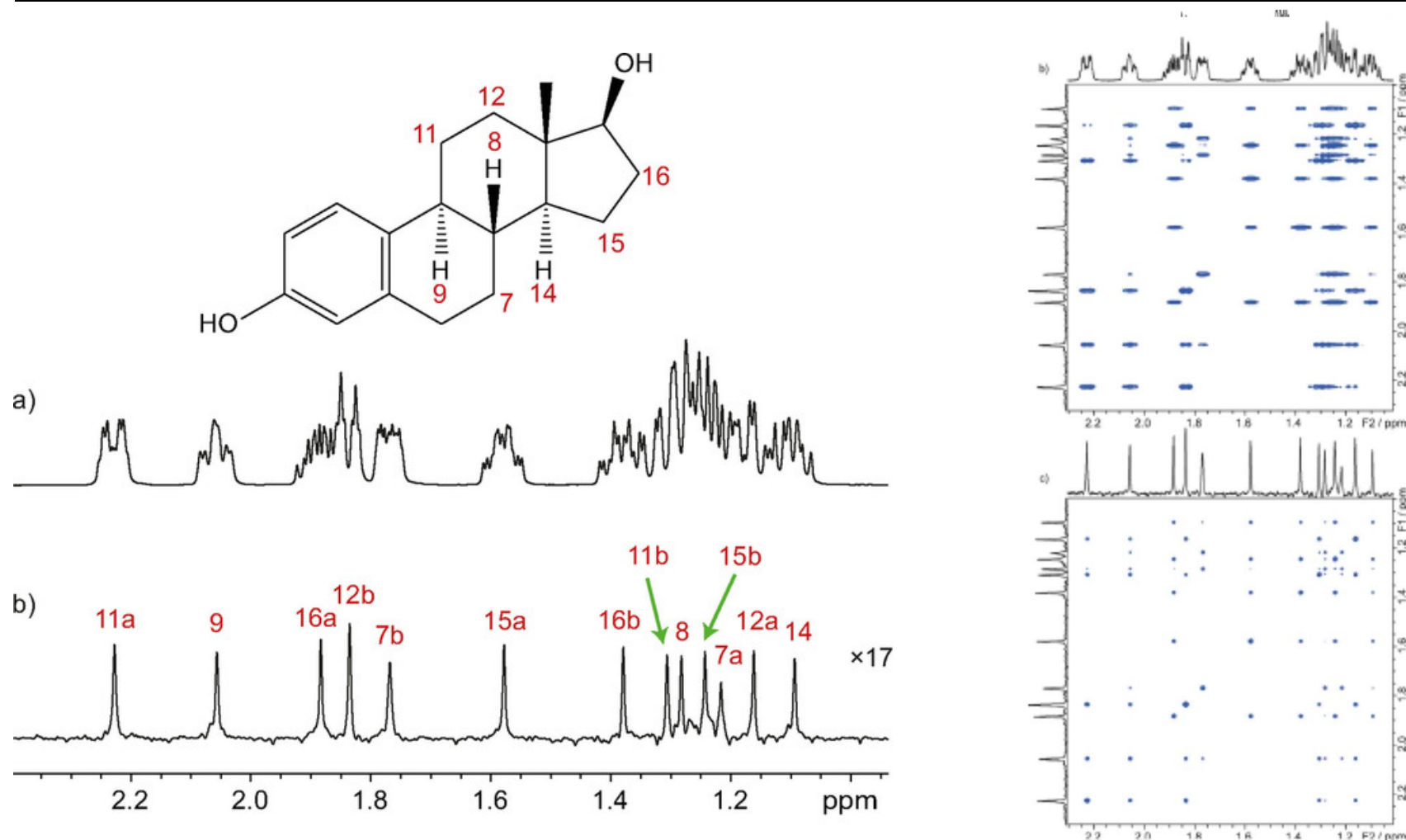
Mixtures: Resolution of Diastereoisomers and Enantiomers



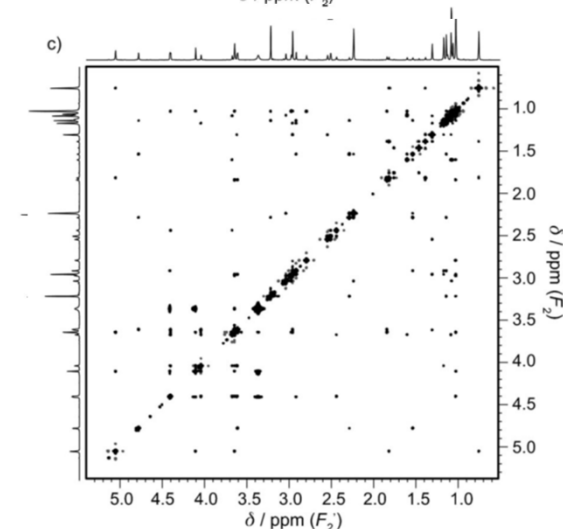
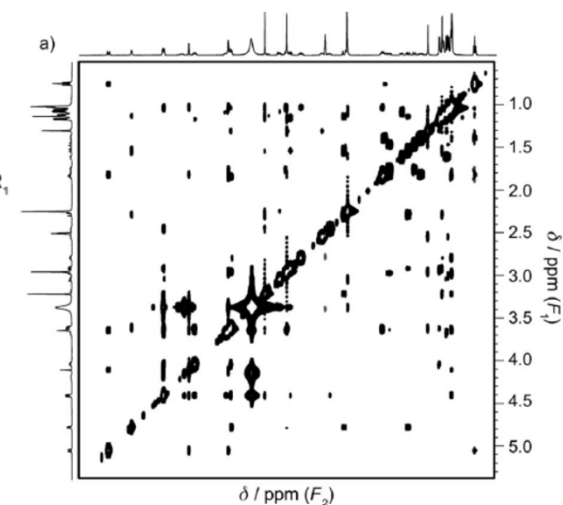
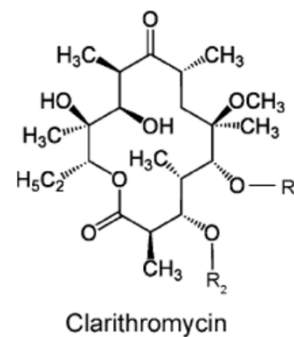
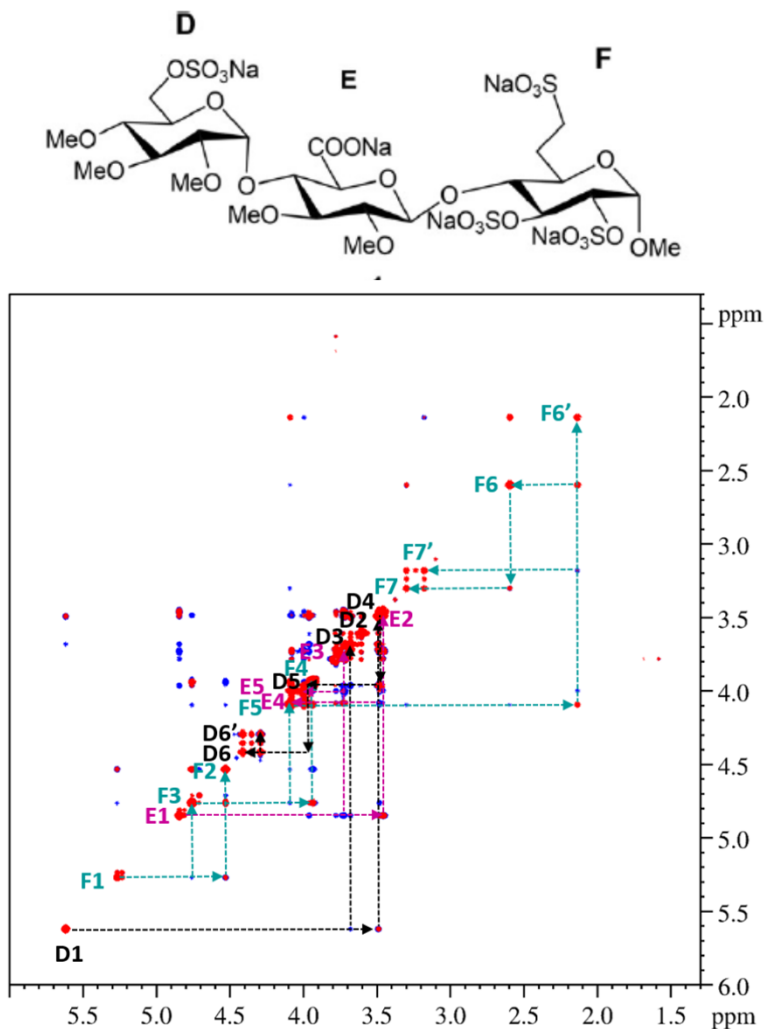
Individual selective spectra (HOBS)



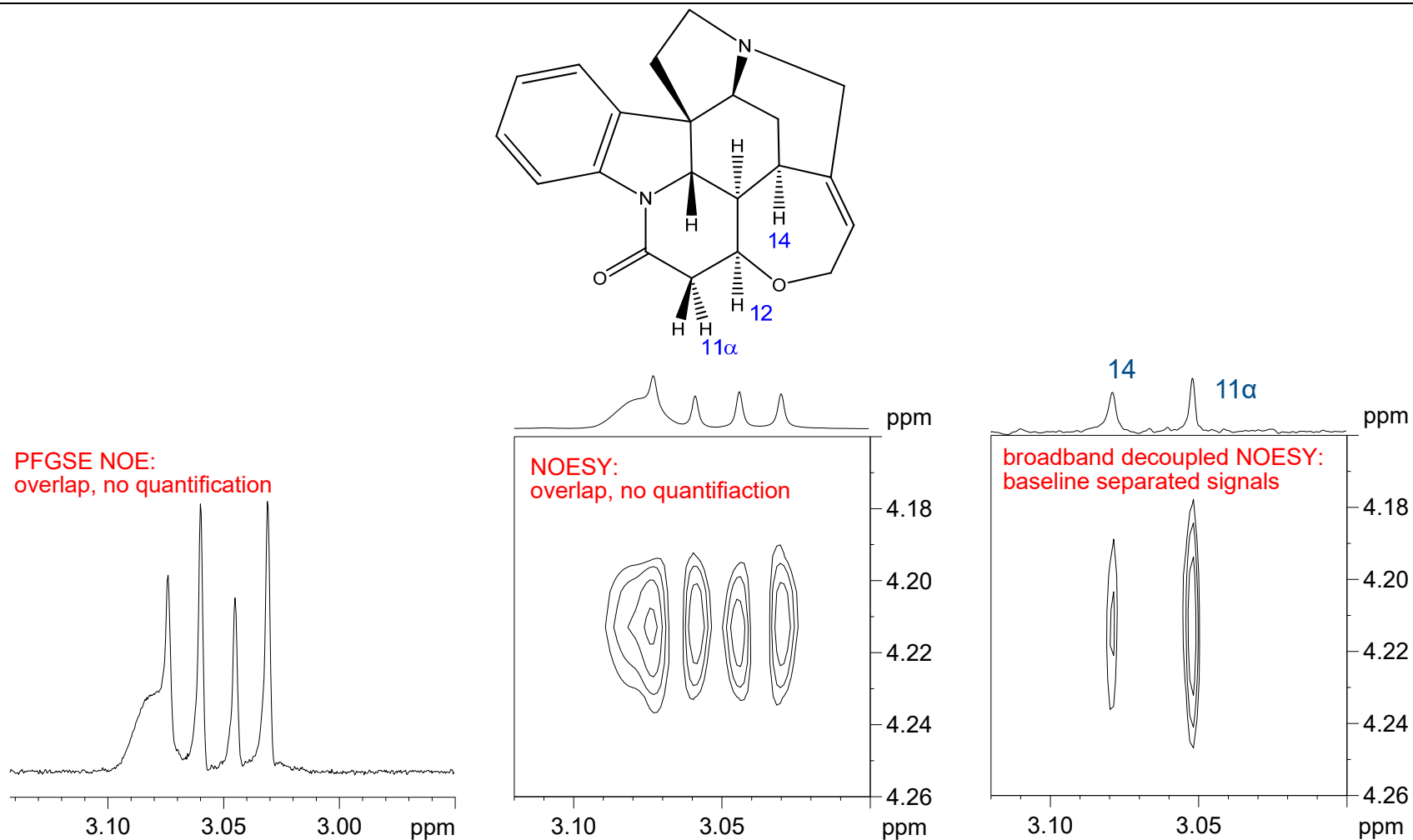
Resolving the resolution problem: overlapped signals in complex compounds: TOCSY



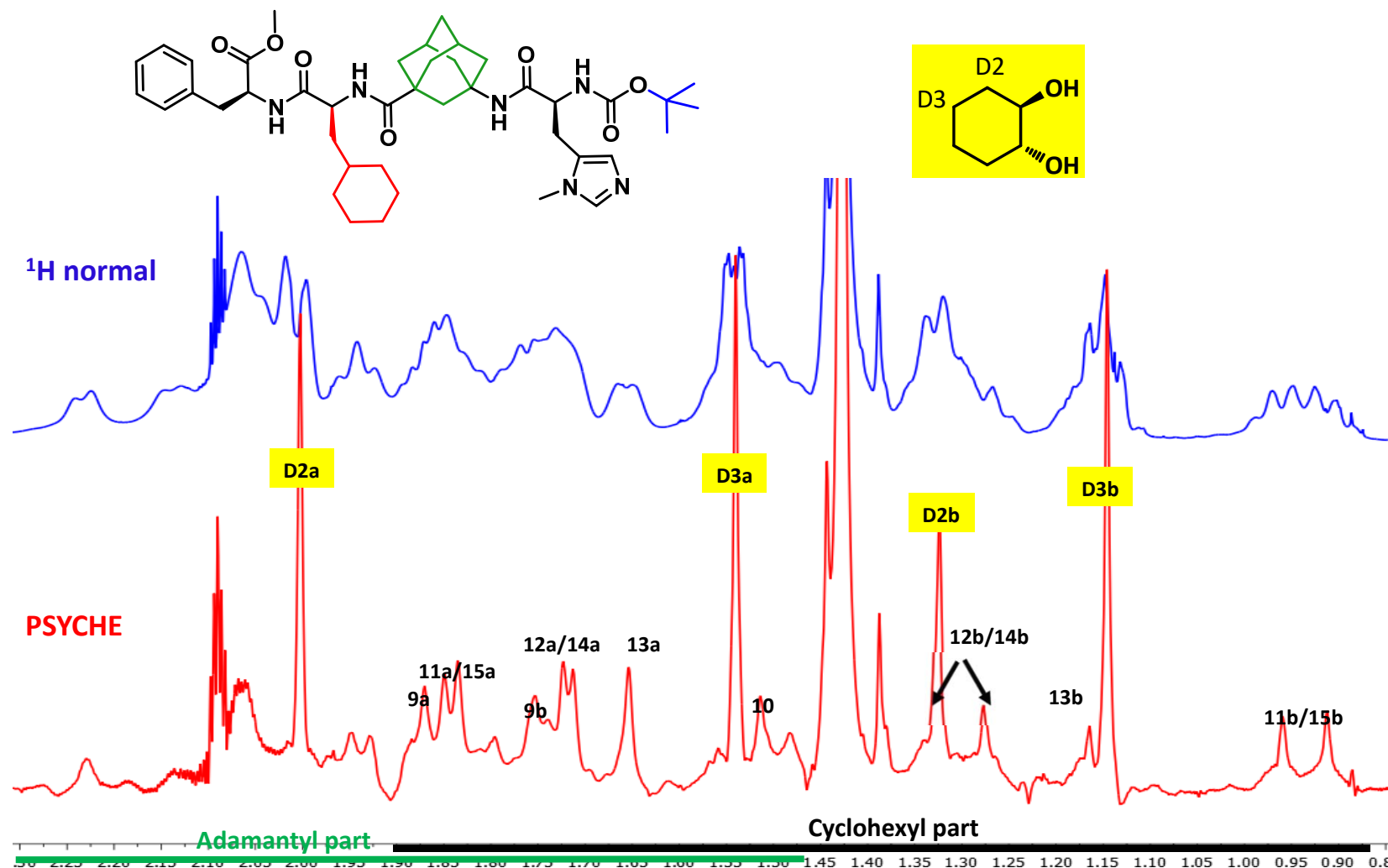
COSY and NOESY



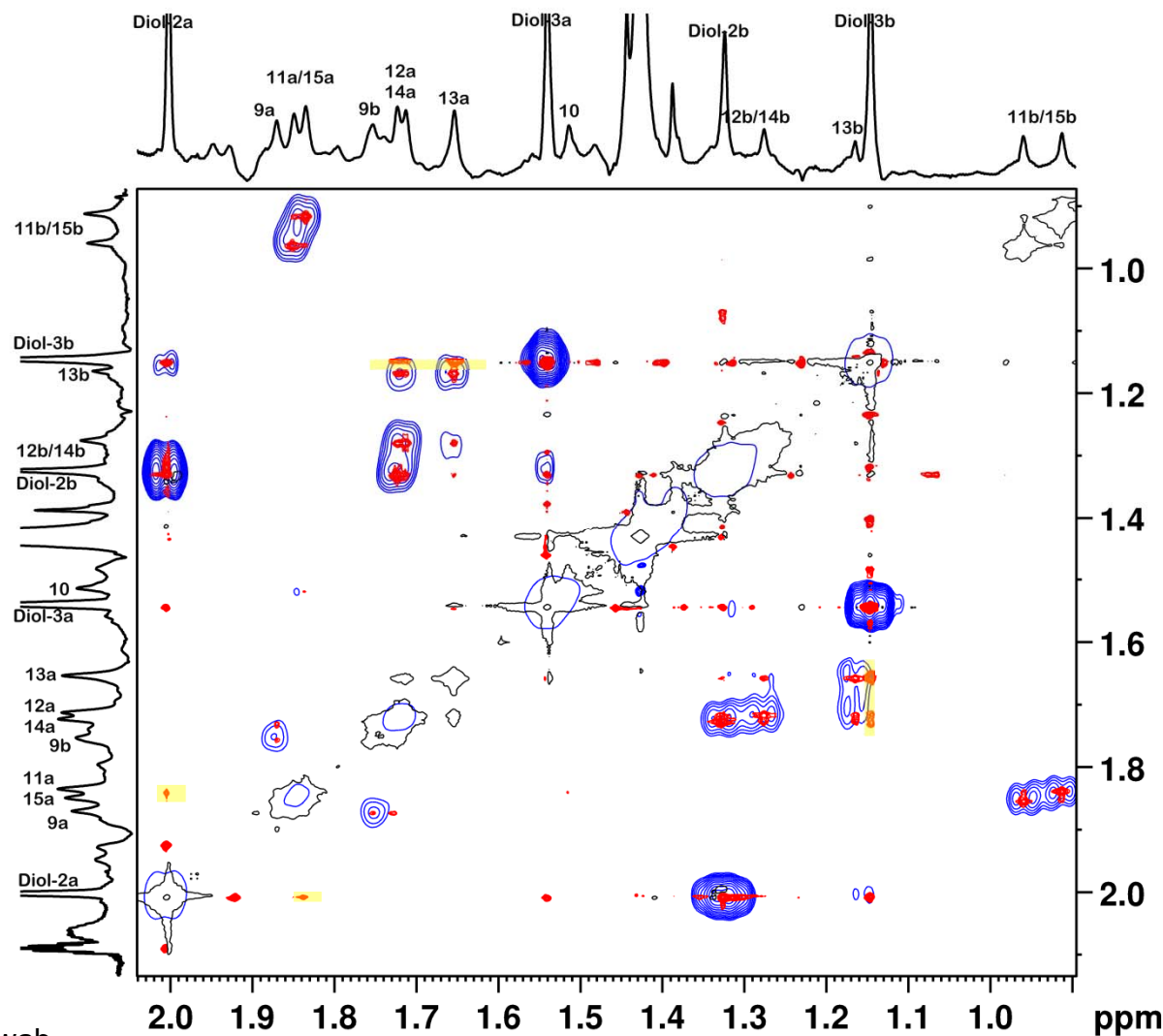
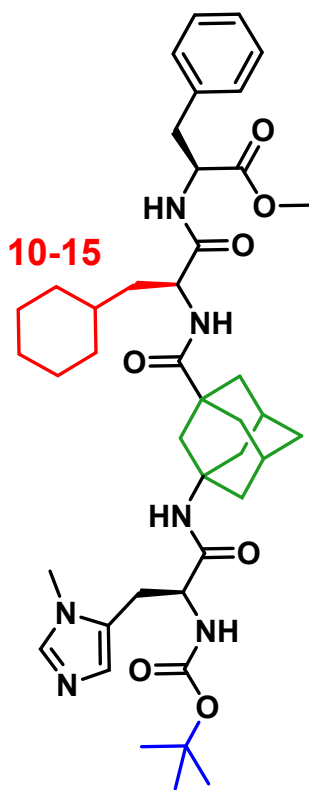
(ZS-)NOESY: Extraction of distance restraints



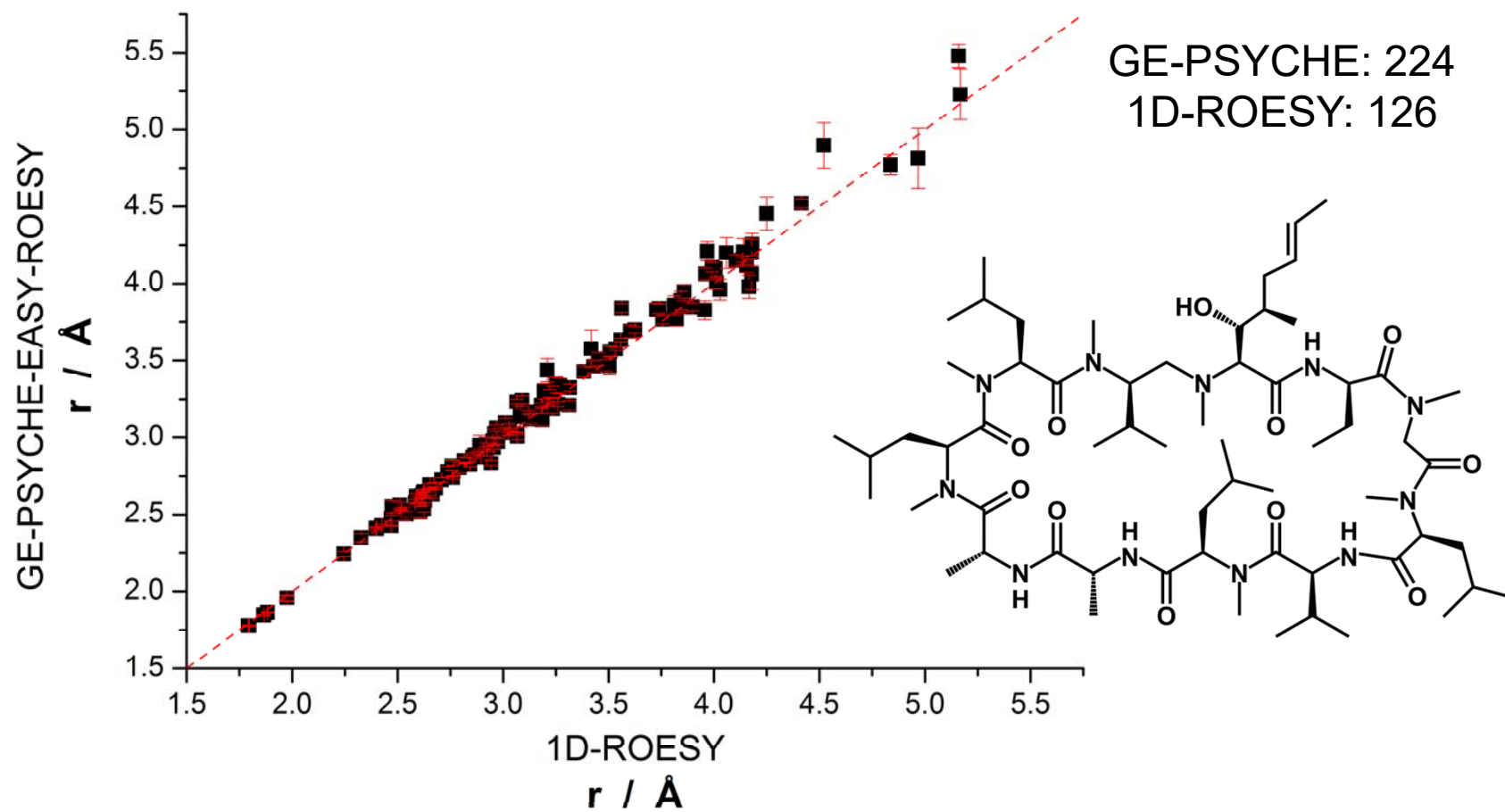
Investigating intermolecular interactions



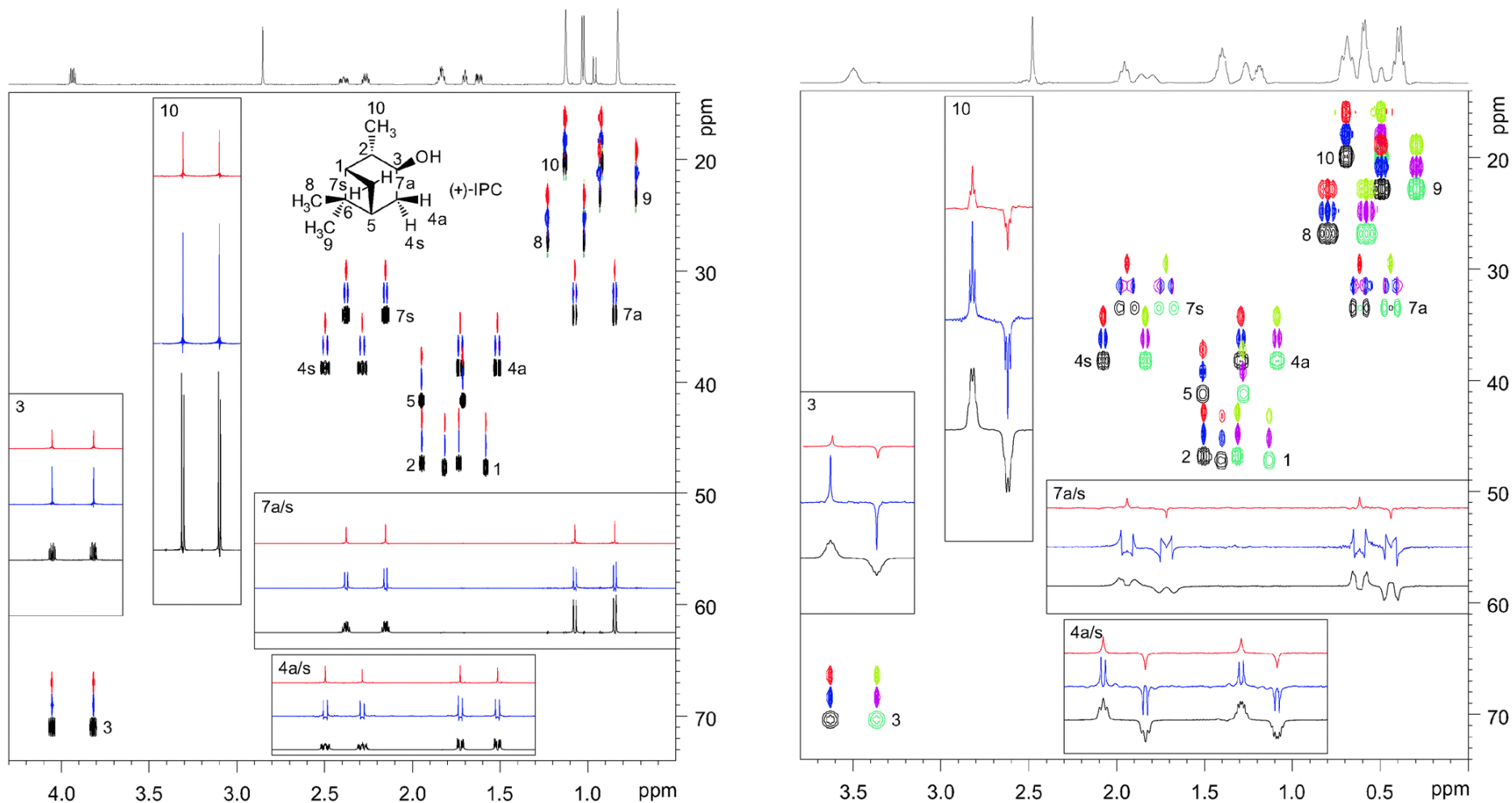
PSYCHE EASY ROESY vs. EASY ROESY



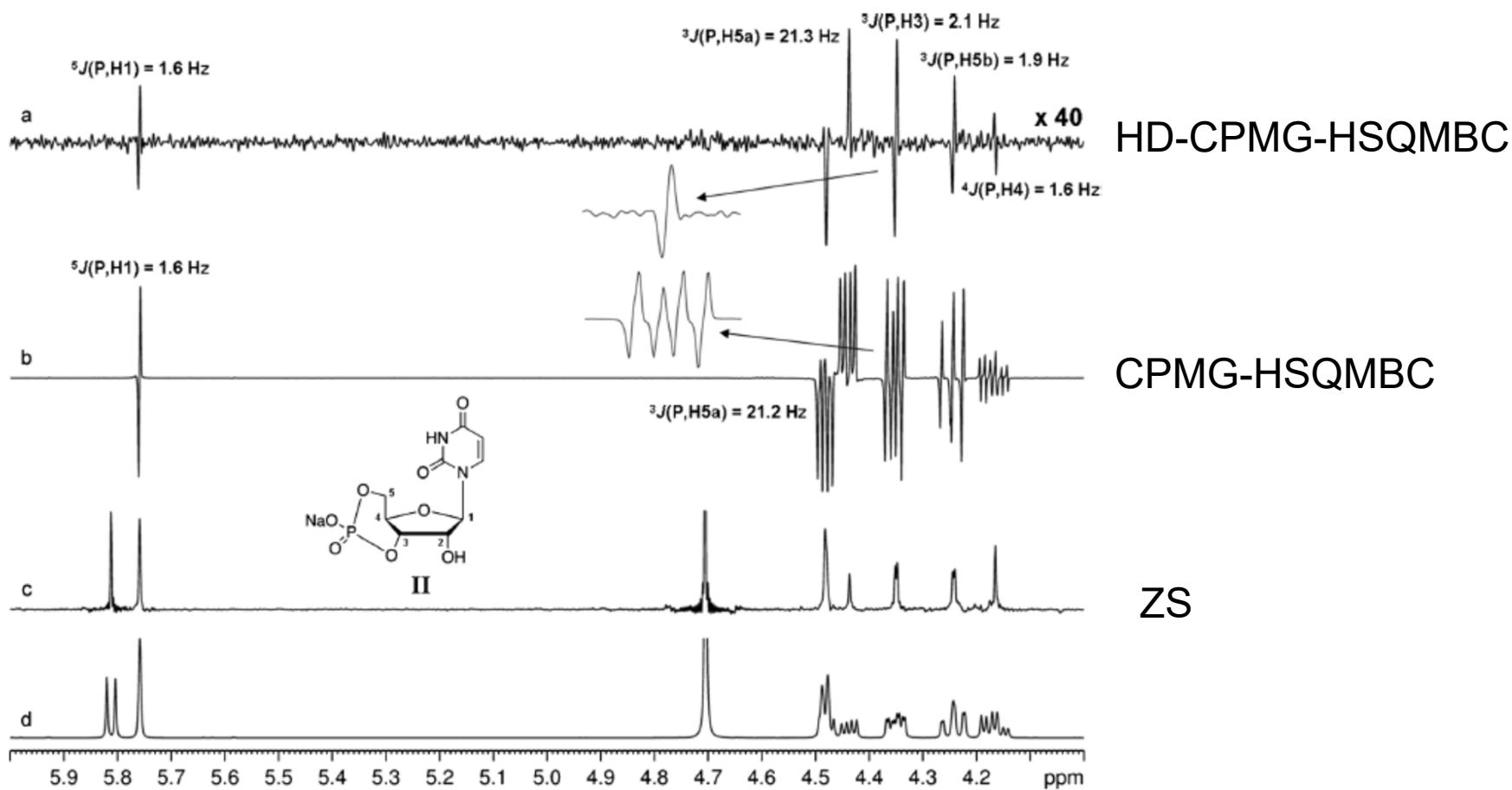
NOEs can be quantified: more distances !



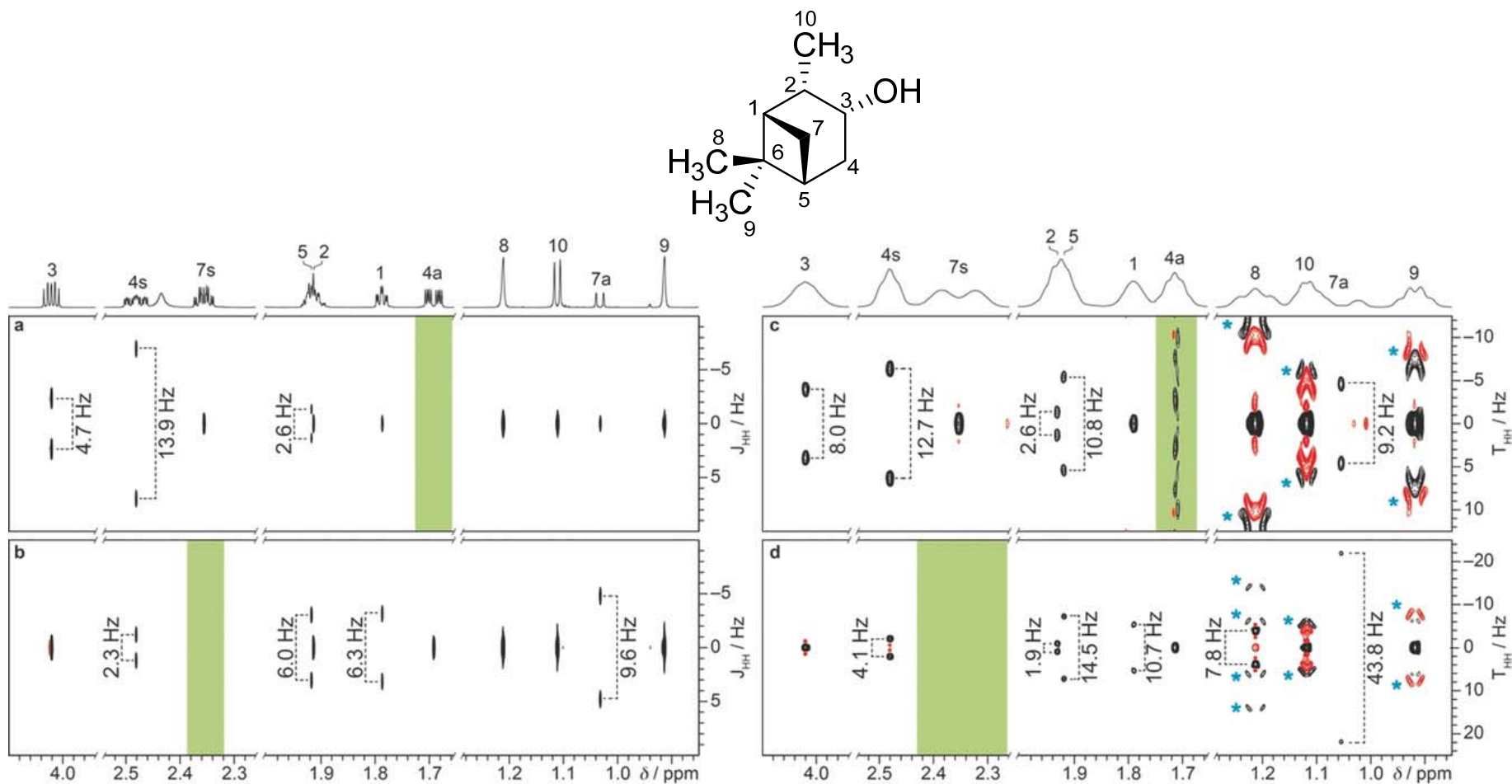
Measurement of one bond couplings /RDCs



Measurement of long-range couplings



Measurement of H-H couplings / RDCs from PSYCHEDELIC

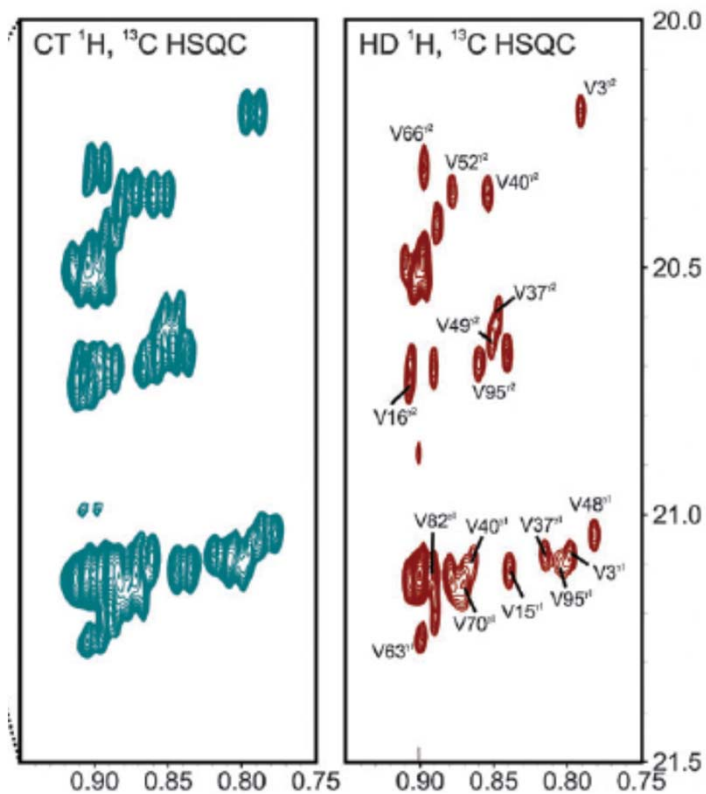


D. Sinnaeve, M. Foroozandeh, M. Nilsson, G. A. Morris, *Angew. Chem. Int. Ed.* **2016**, *55*, 1090

D. Sinnaeve, J. Ilgen, M. E. Di Pietro, J. J. Primozic, V. Schmidts, C. M. Thiele, B. Luy, *Angew. Chem. Int. Ed.* **2020**, *59*, 5316-5320

What about (intrinsically disordered) proteins ?

CT vs. ZS-HSQC of α -Synuclein



CT (a) vs. SHACA-HSQC (d) of transactivation domain of p53

