Problem of the Month:

May 2021

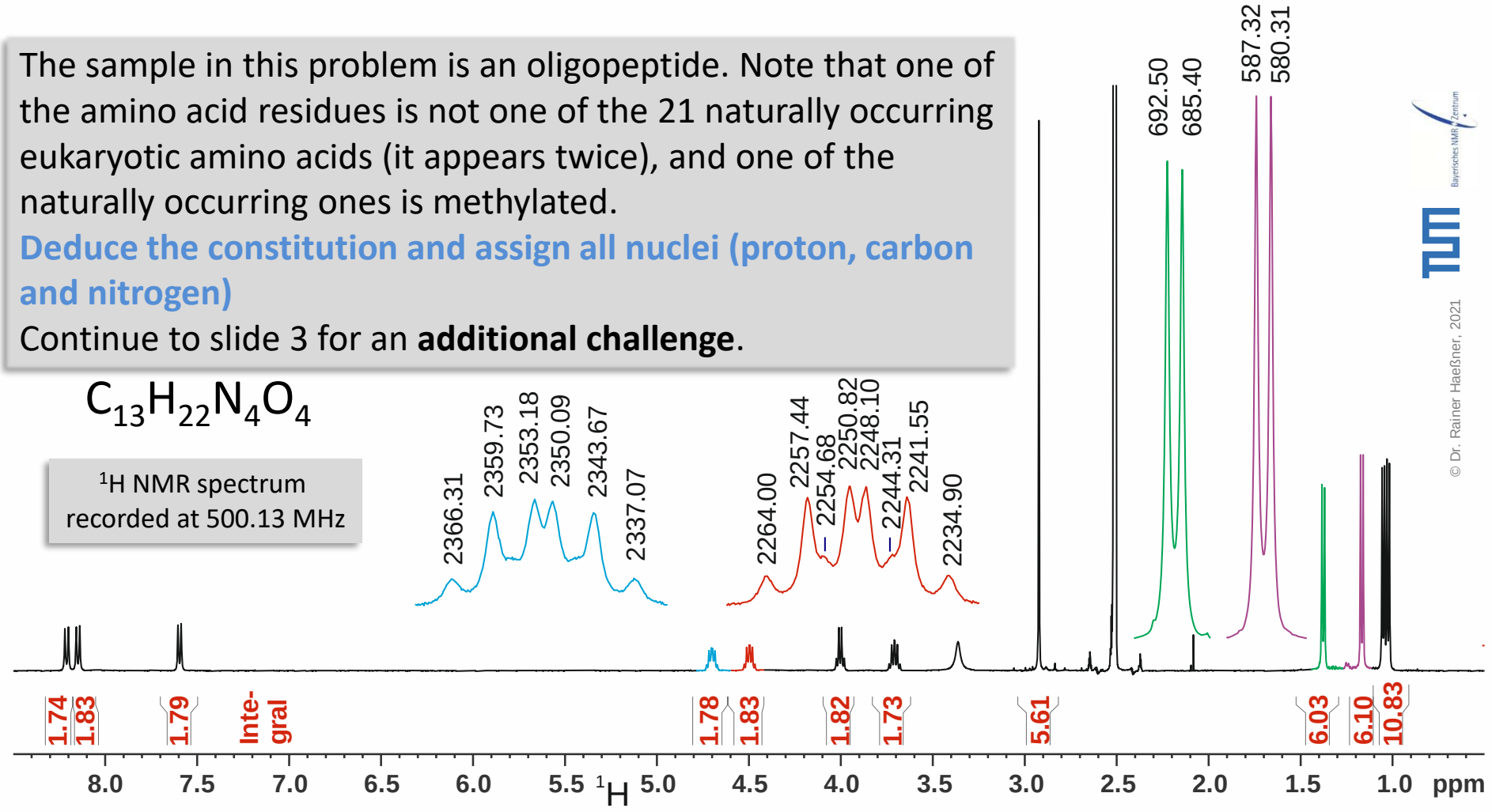
The sample in this problem is an oligopeptide. Note that one of the amino acid residues is not one of the 21 naturally occurring eukaryotic amino acids (it appears twice), and one of the naturally occurring ones is methylated.

Deduce the constitution and assign all nuclei (proton, carbon and nitrogen)

Continue to slide 3 for an **additional challenge**.

$C_{13}H_{22}N_4O_4$

^{1}H NMR spectrum recorded at 500.13 MHz

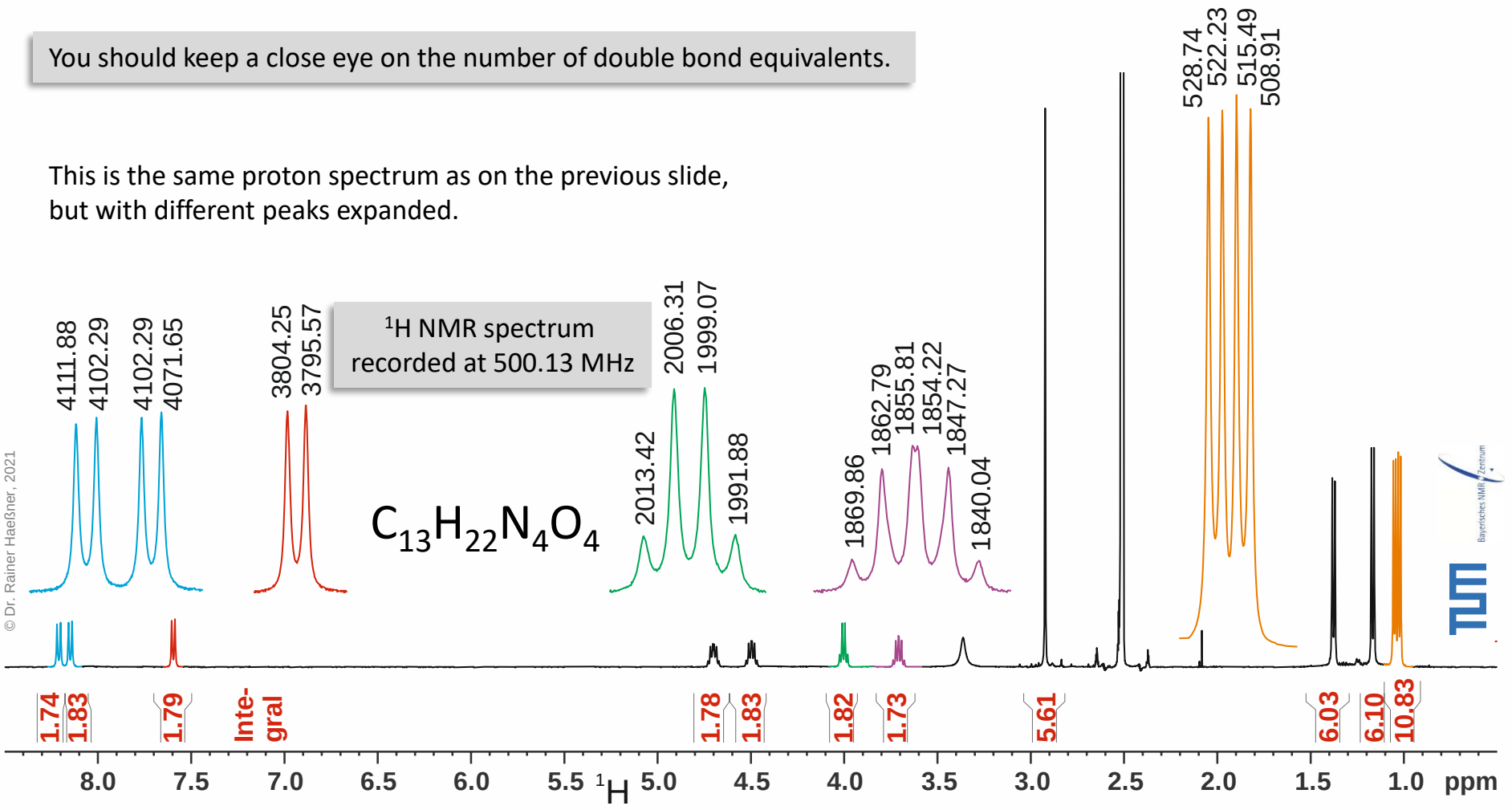


Problem of the Month:

May 2021

You should keep a close eye on the number of double bond equivalents.

This is the same proton spectrum as on the previous slide, but with different peaks expanded.

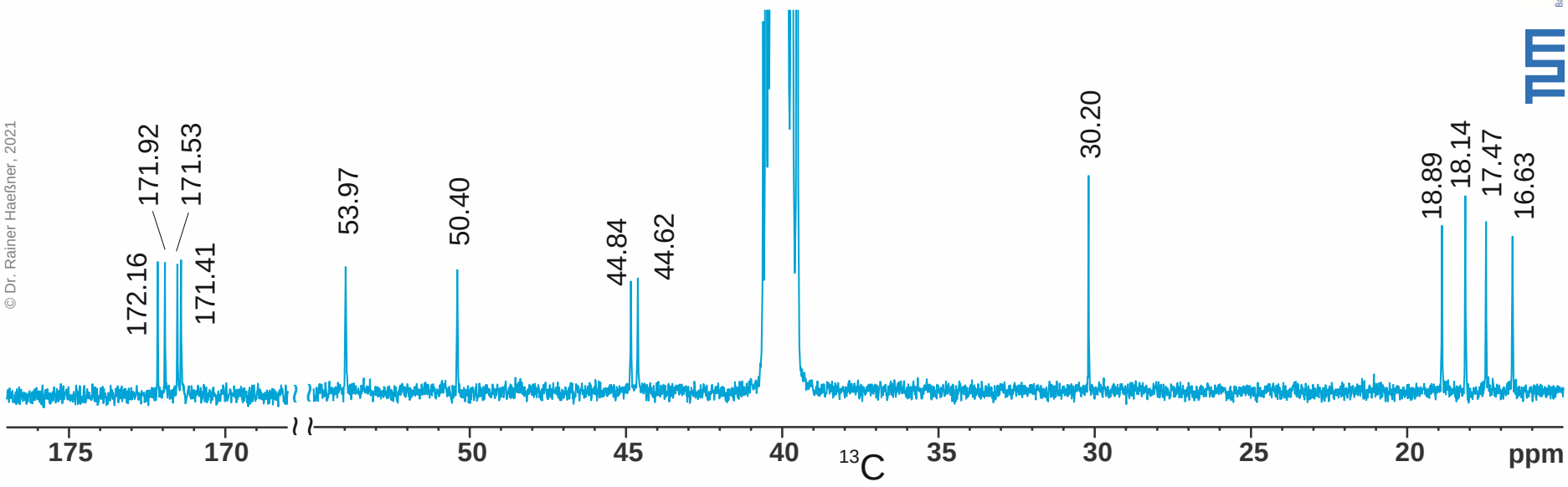


Problem of the Month:

May 2021

Extra challgenge: If you have access to molecular modeling software, you might try to extract pieces of information about the absolute configuration (e.g. NOESY).

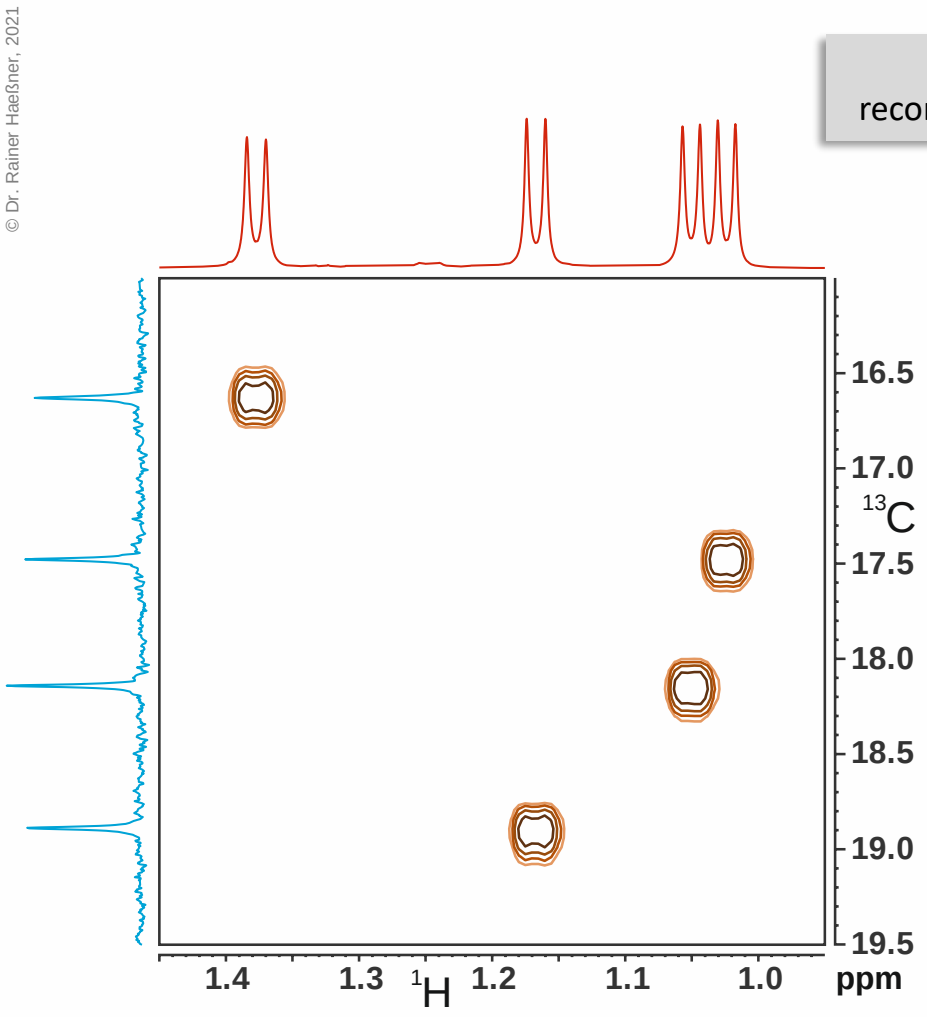
$^{13}C\{^{1}H\}$ NMR spectrum
recorded at 125.80{500.13} MHz

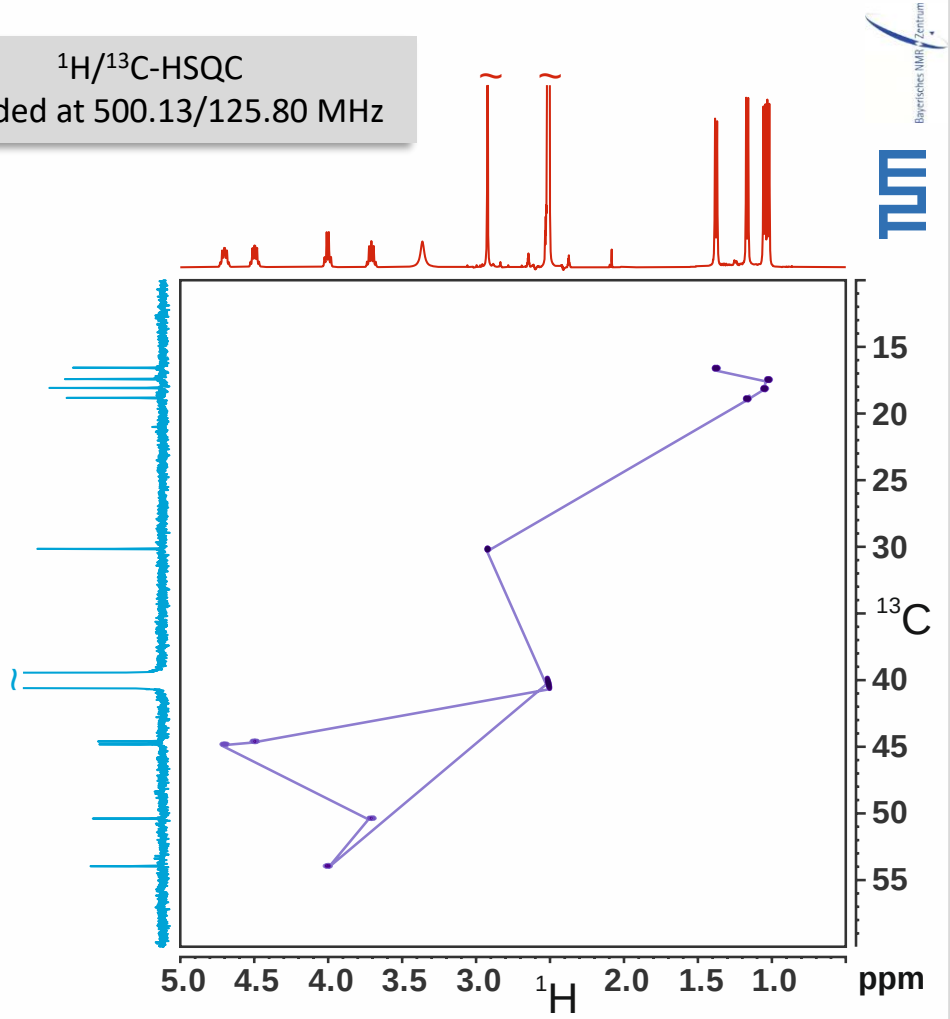


Problem of the Month:

May 2021

$^{1}H/^{13}C$-HSQC
recorded at 500.13/125.80 MHz

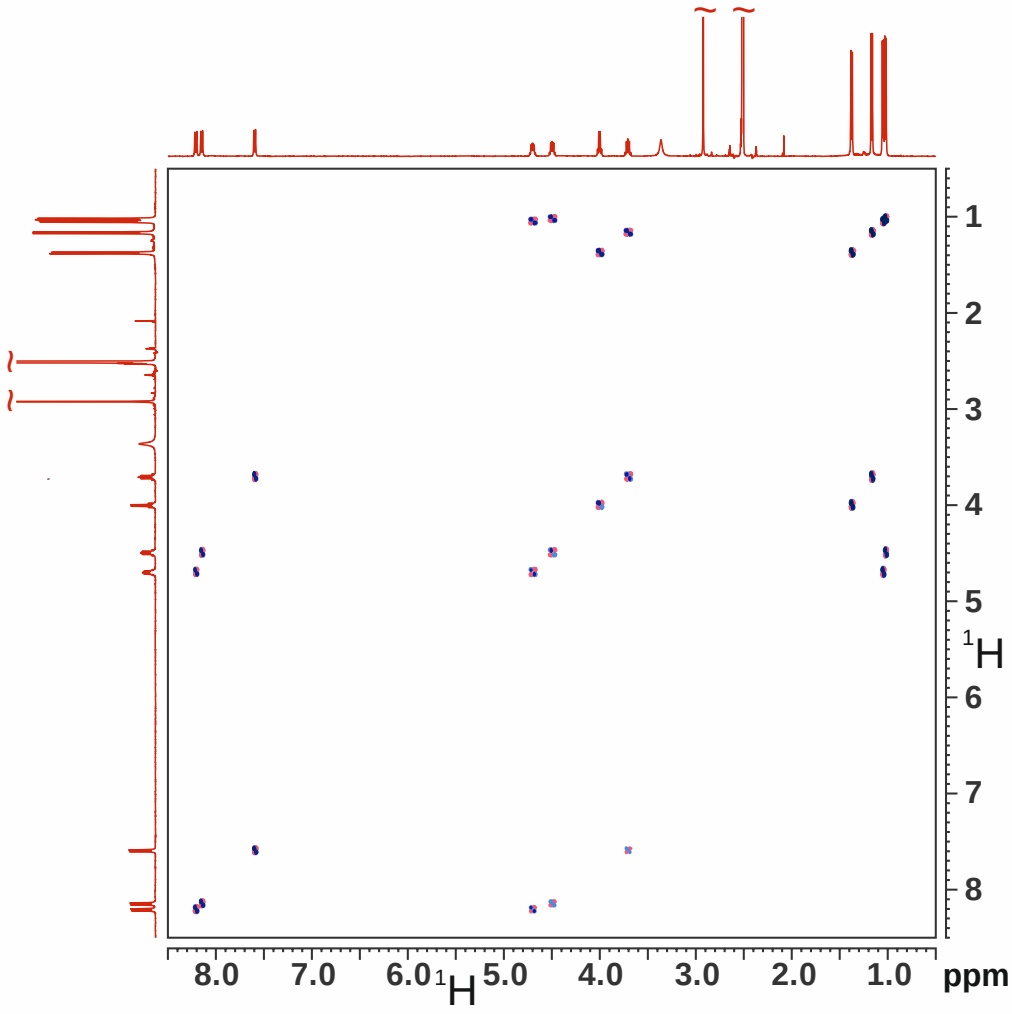




Problem of the Month:

May 2021

$^{1}H/^{1}H$-COSY
recorded at 500.13 MHz

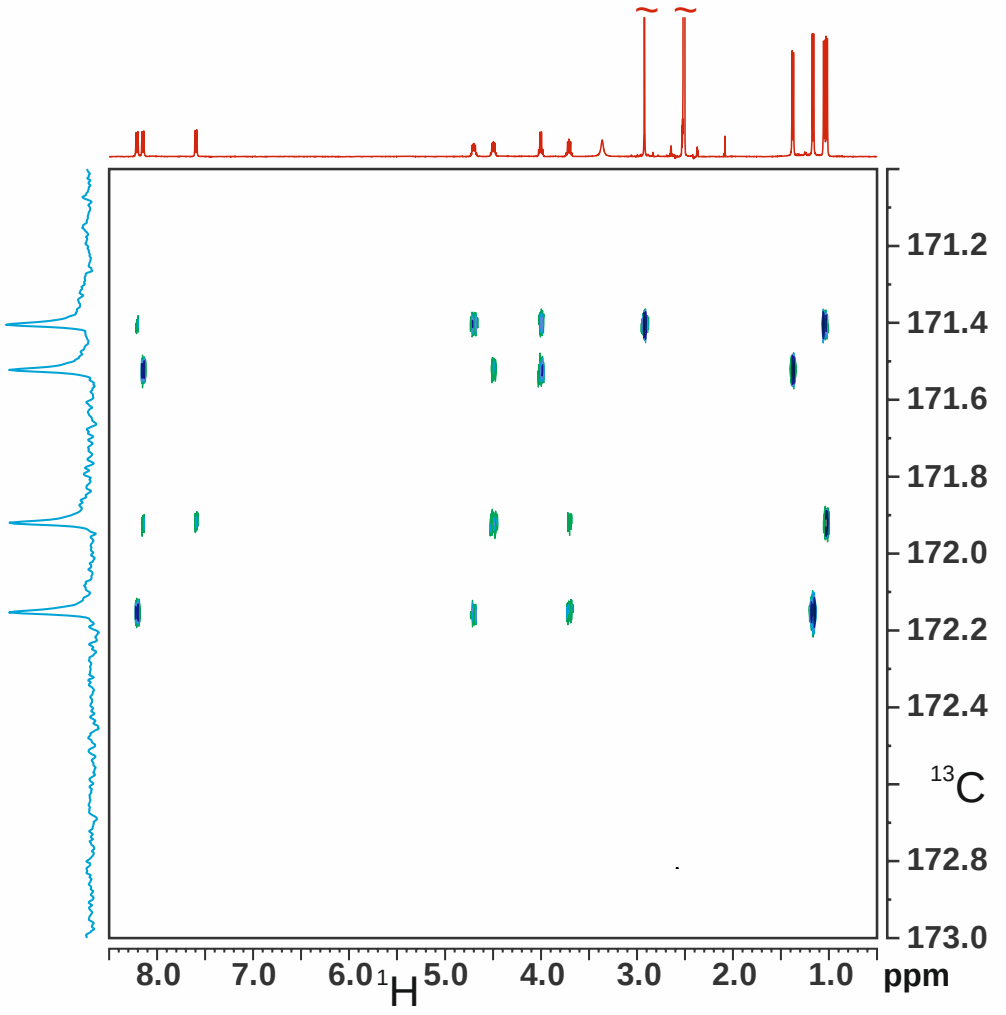


Bayerisches NMR Zentrum

Problem of the Month:

May 2021

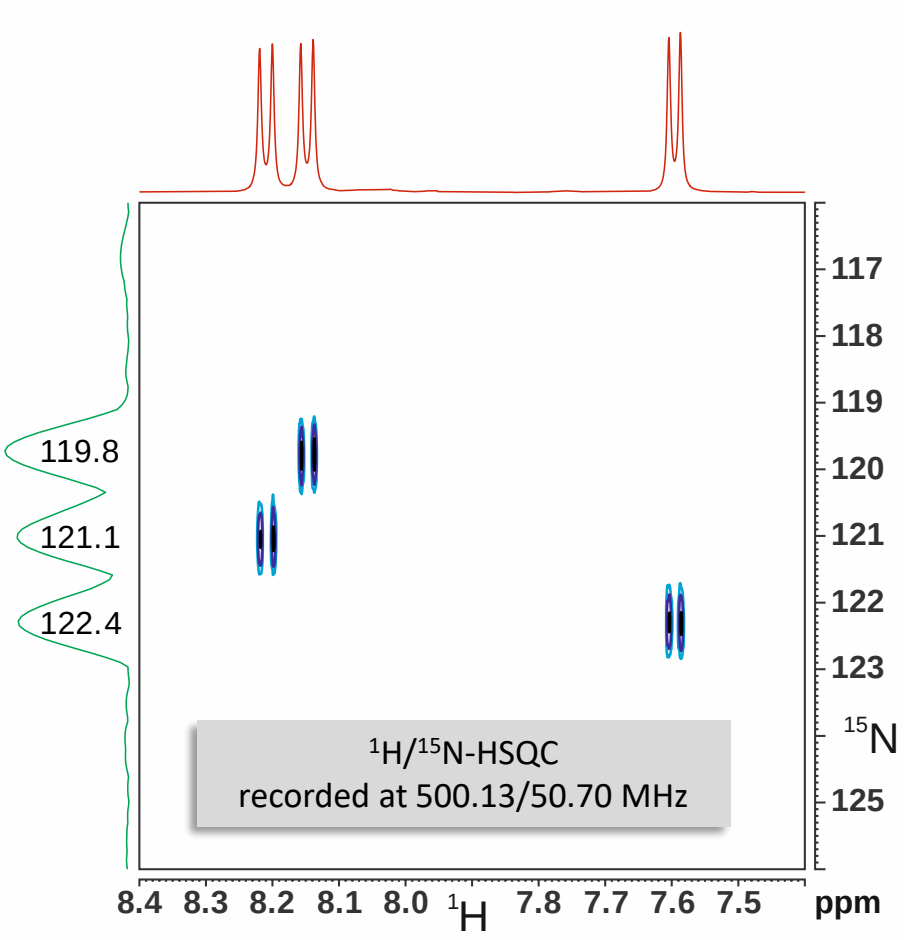
expansion of $^{1}H/^{13}C$-HMBC
recorded at 500.13/125.80 MHz

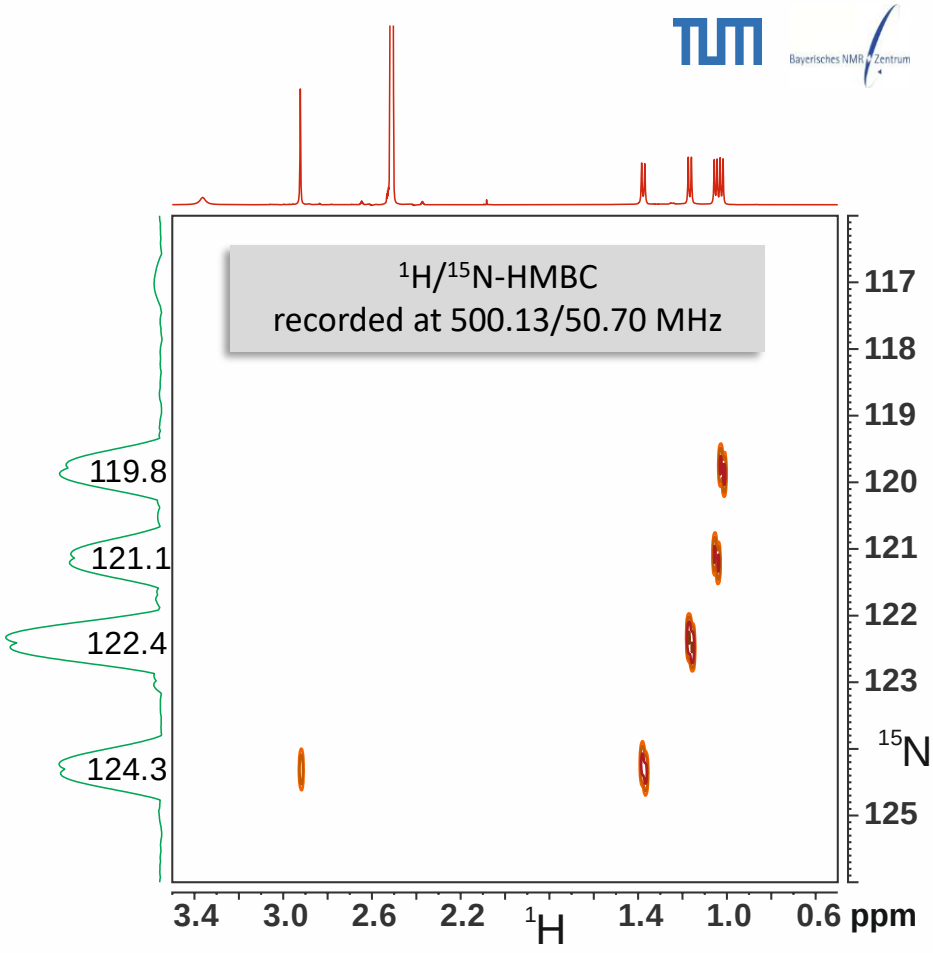


Bayerisches NMR Zentrum

Problem of the Month:

May 2021





Problem of the Month:

May 2021

expansion of $^{1}H/^{1}H$-NOESY
recorded at 500.13 MHz

(true NOESY peaks are displayed in red)