

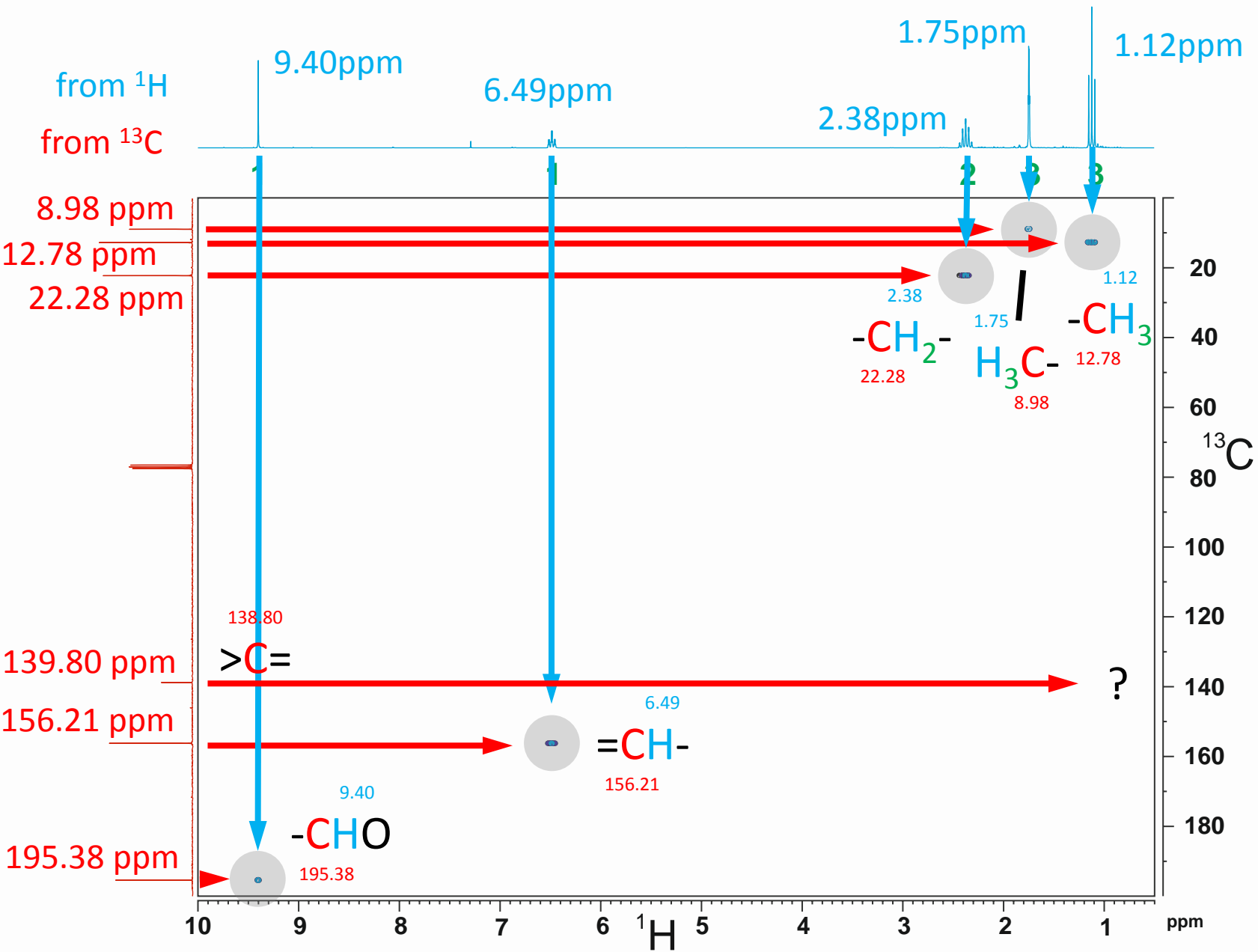
# Problem of the Month:

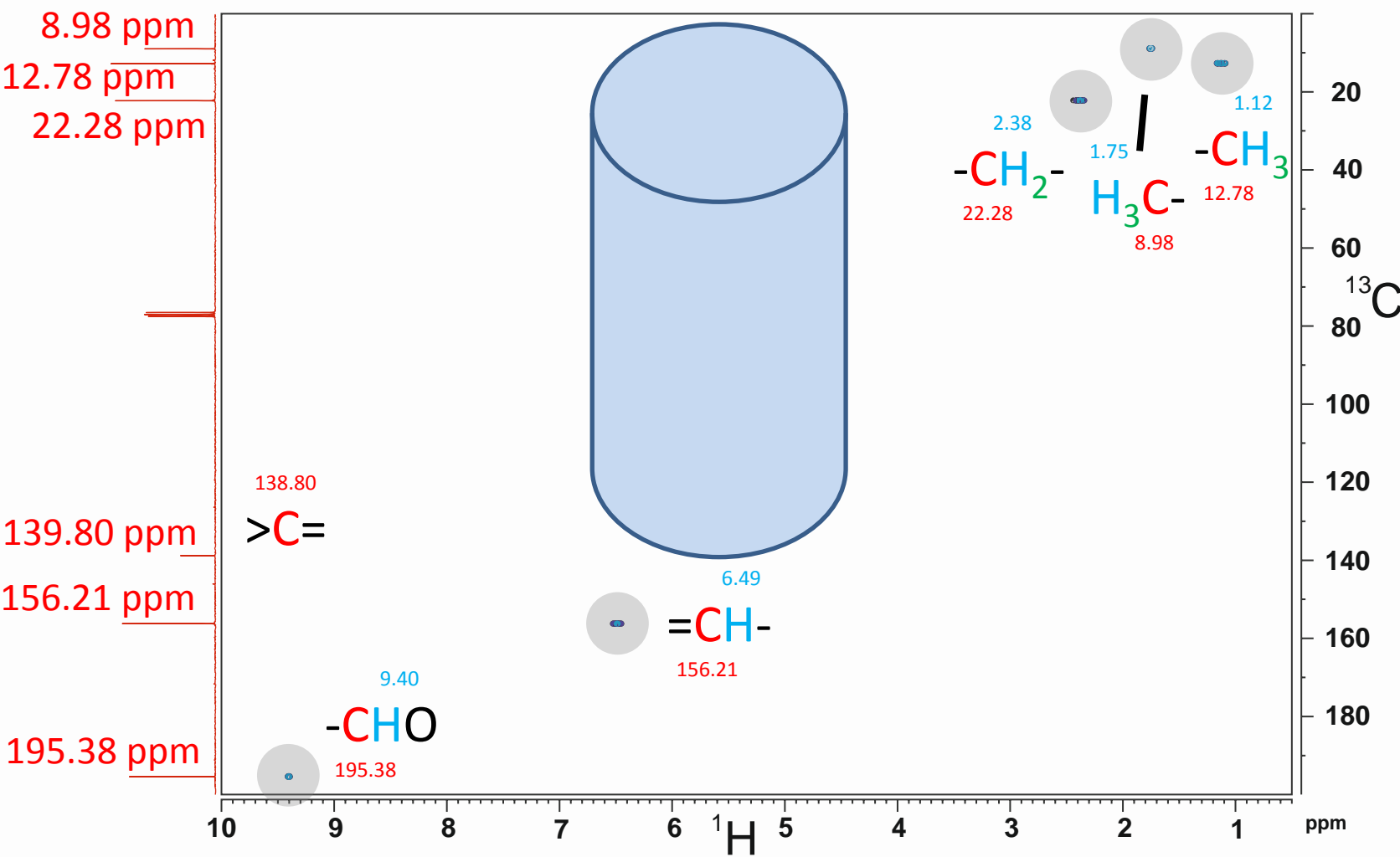
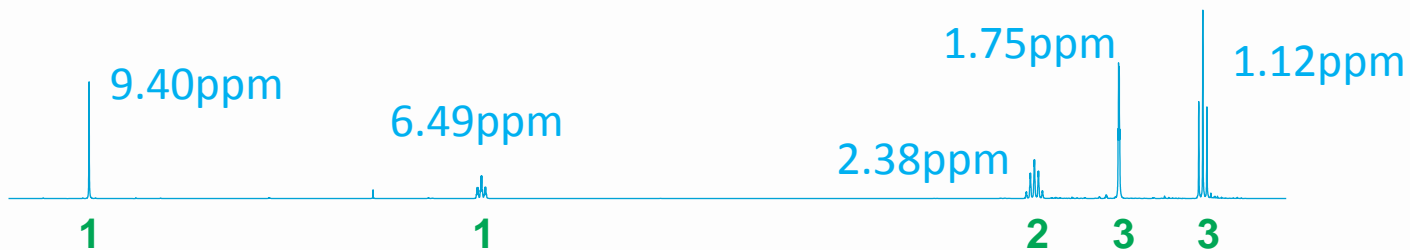
February 2020

# Solution

## Step 1

- (1) Integrate the proton spectrum.
- (2) Transfer the integral values to the proton projection of the HSQC
- (3) Get the building blocks from the HSQC cross peaks





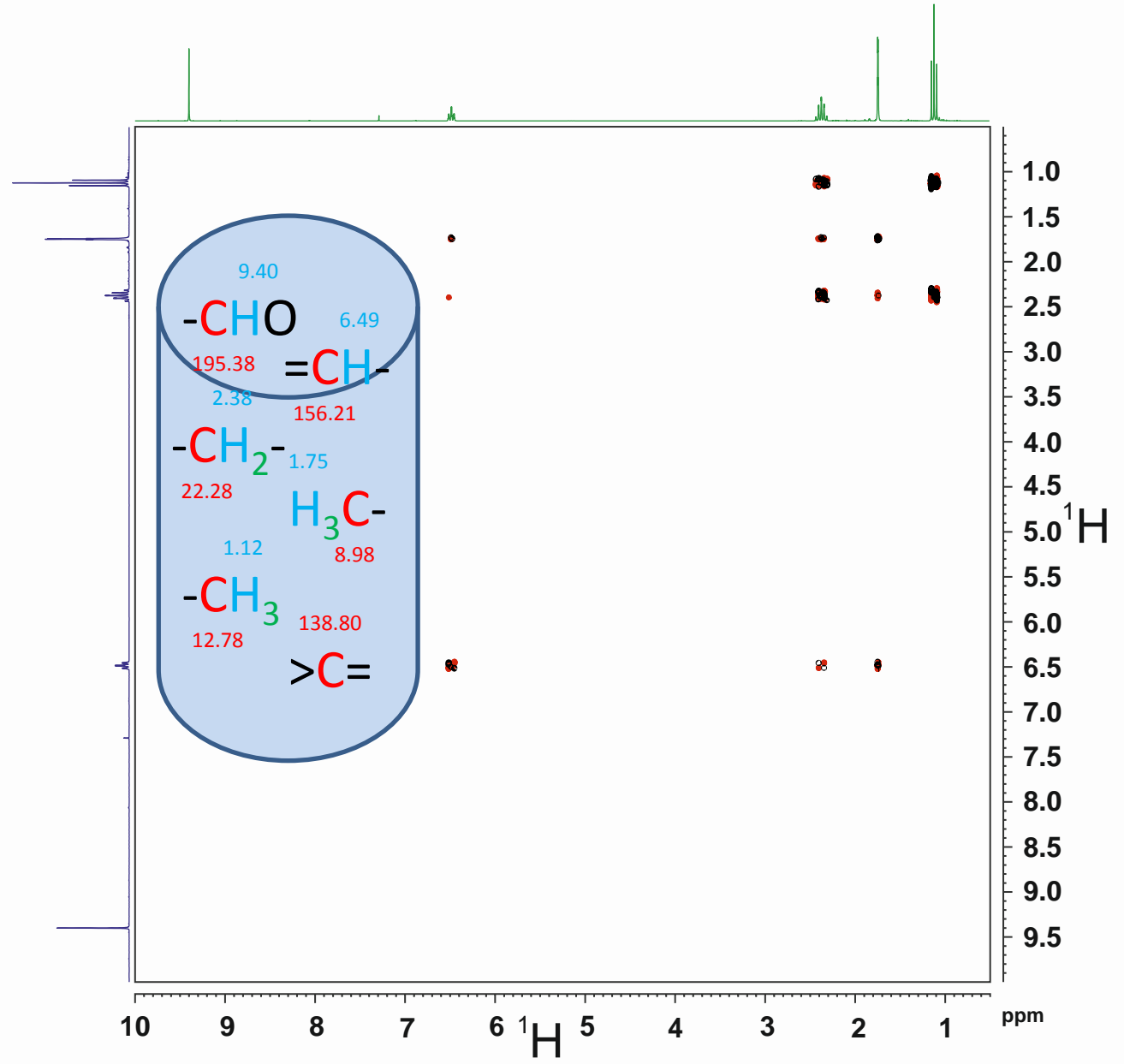
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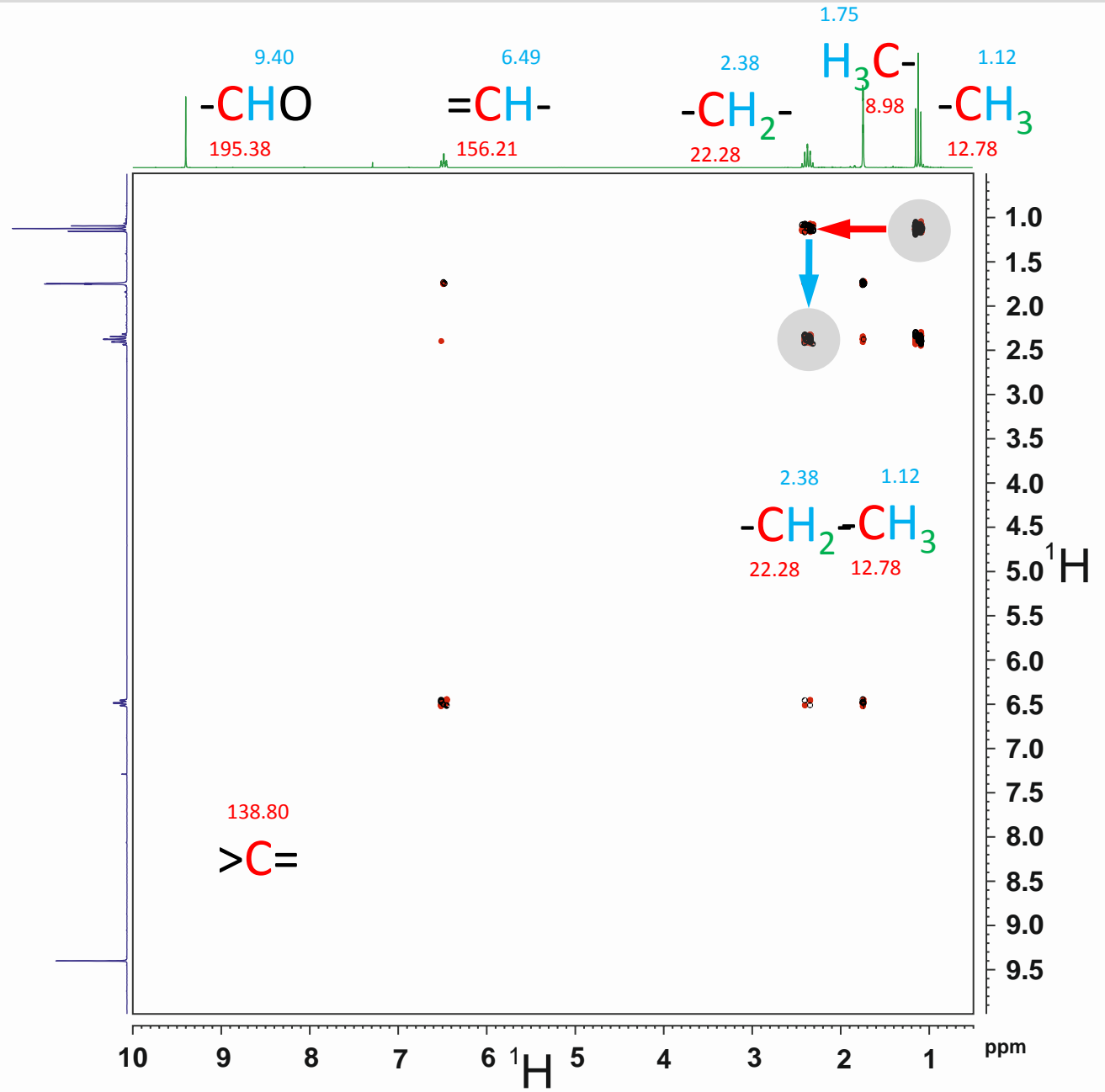
February 2020

# Solution

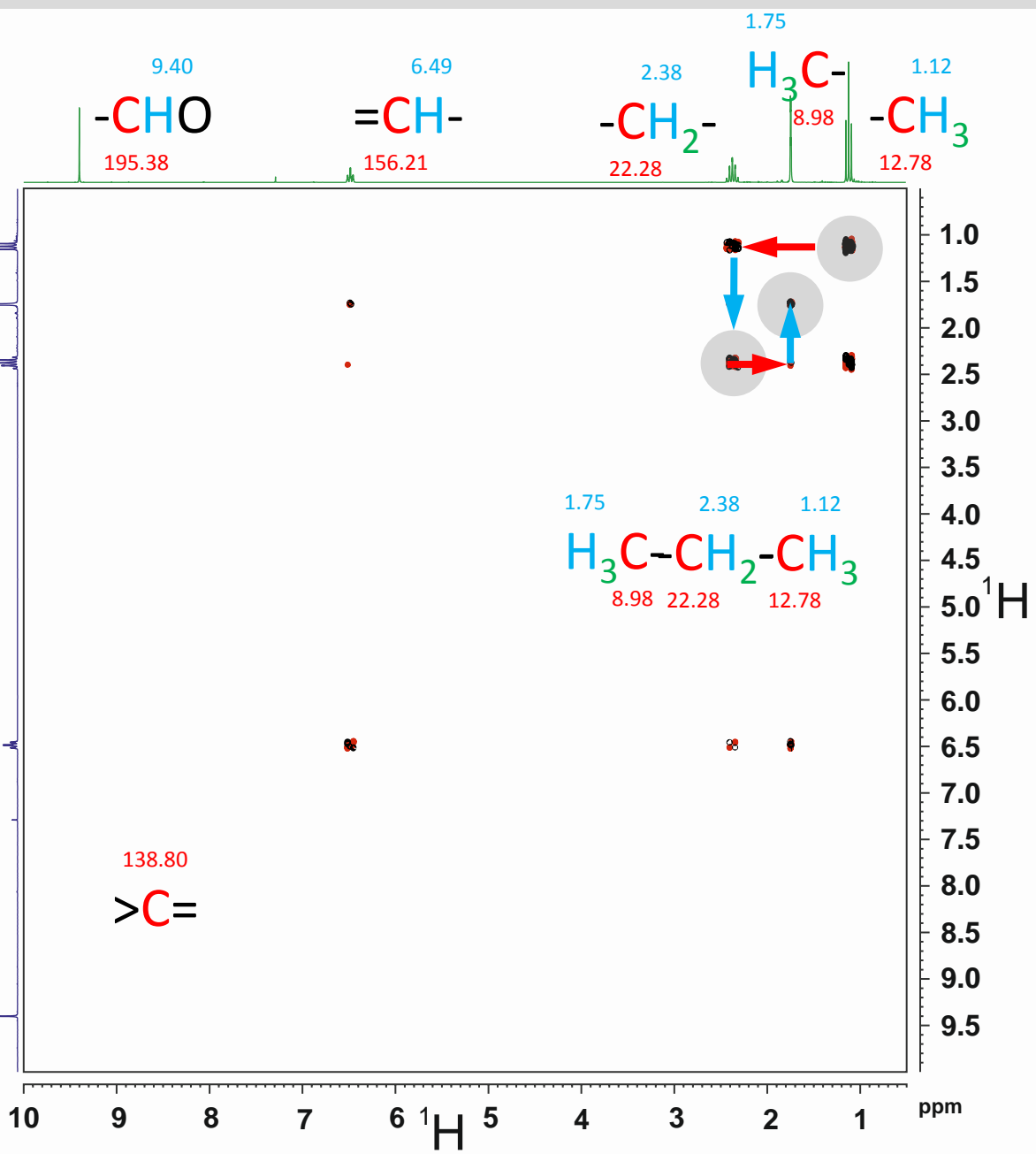
## Step 2

- (1) Connect individual building blocks through COSY correlations.
- (2) Explain multiplet structure of all splittings visible in  $^1\text{H}$  NMR spectrum
- (3) To back up your assumptions you may finally control correlations in HMBC experiment



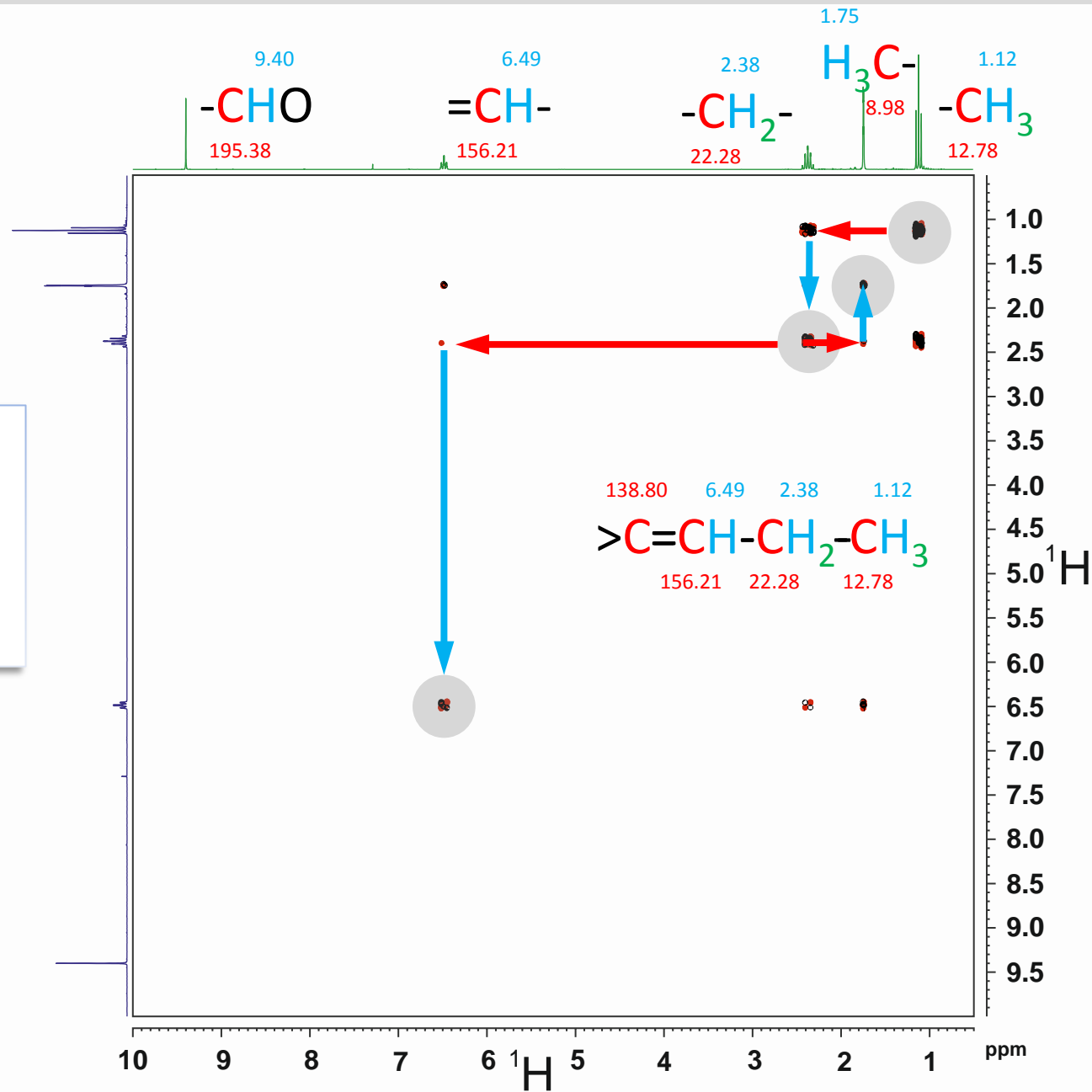


**Really?**  
 And the remaining unassigned groups?



Bayerisches NMR Zentrum

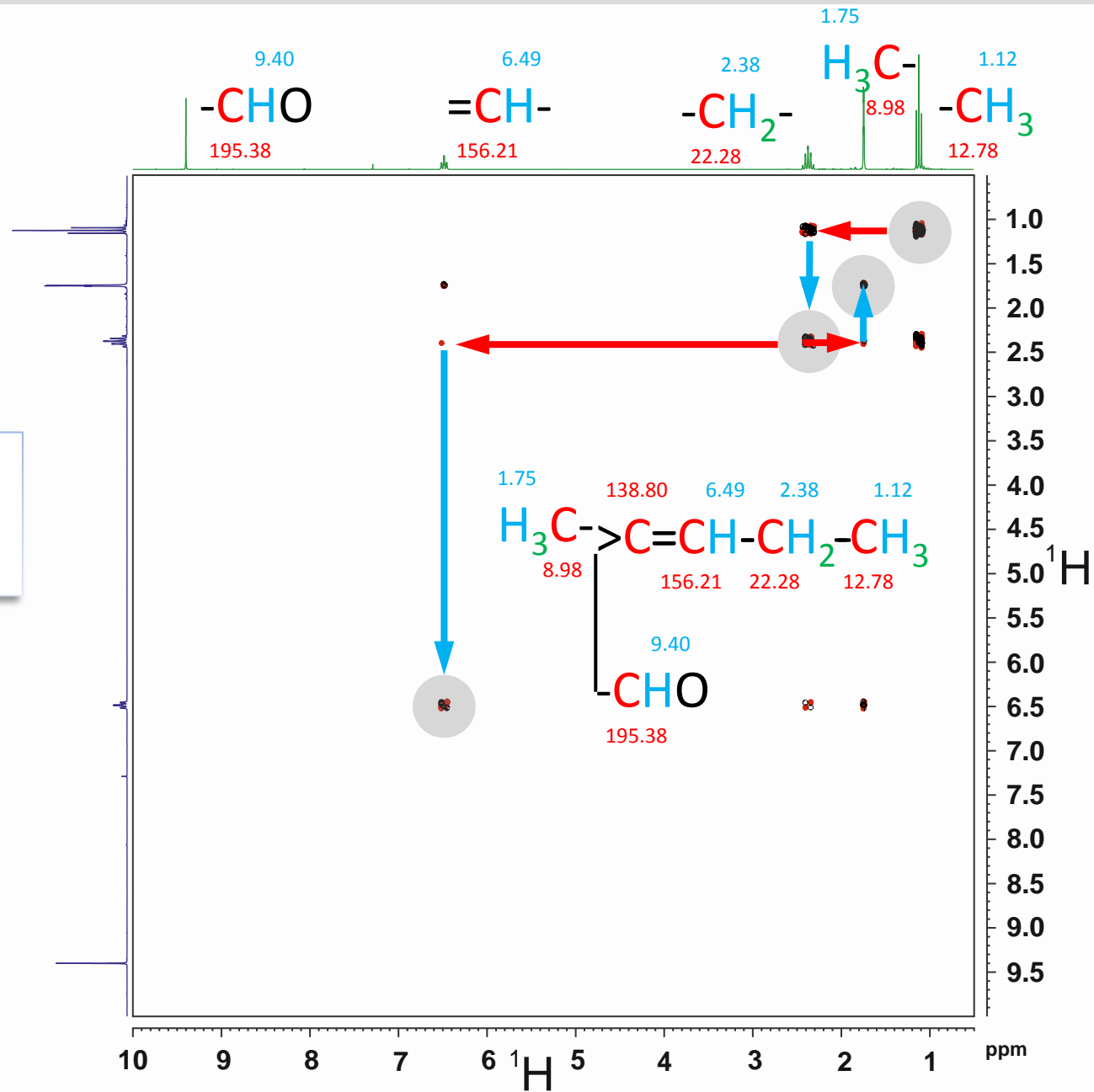
**Why?**  
 There is no other fragment with double bond





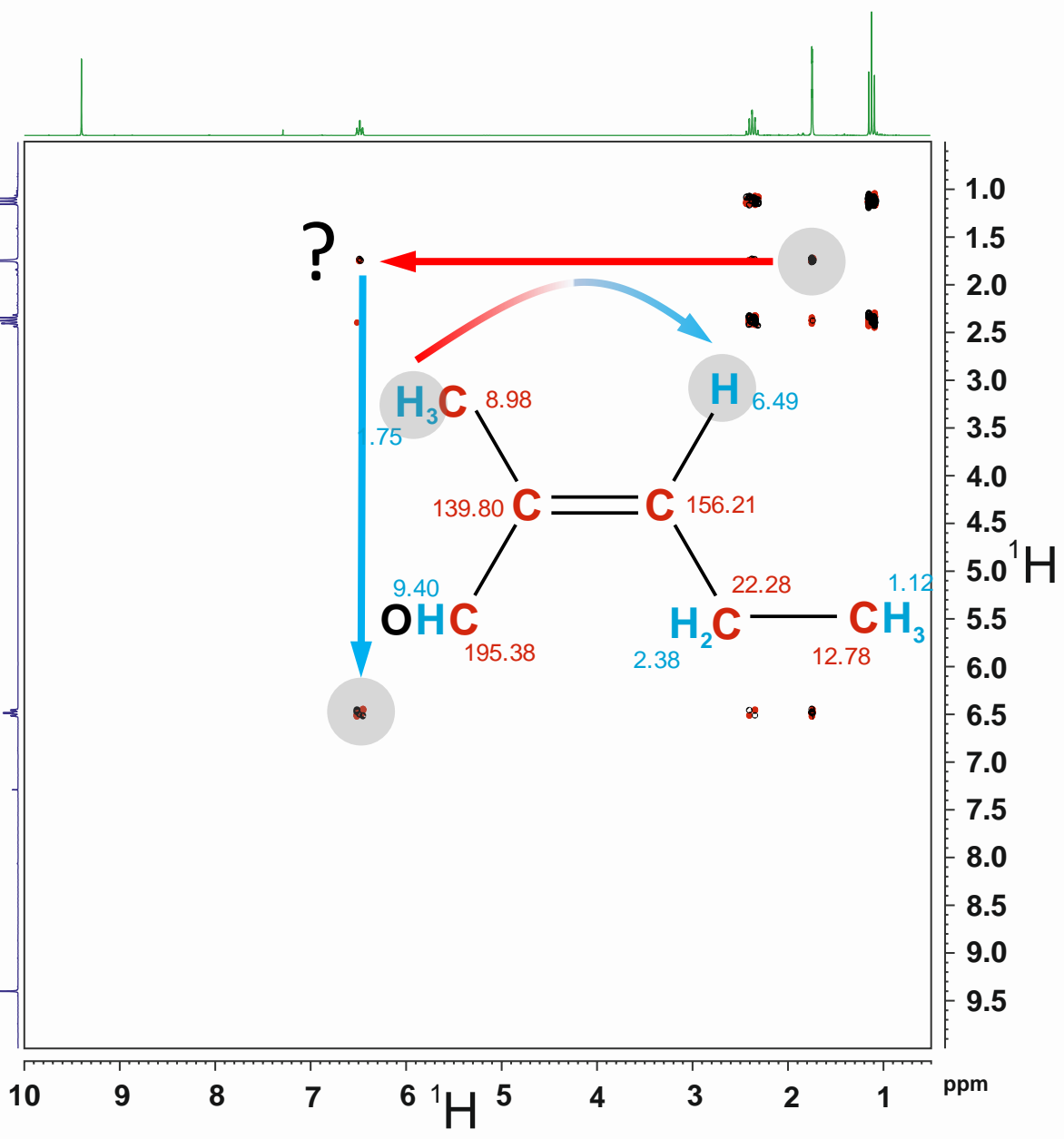
Why?

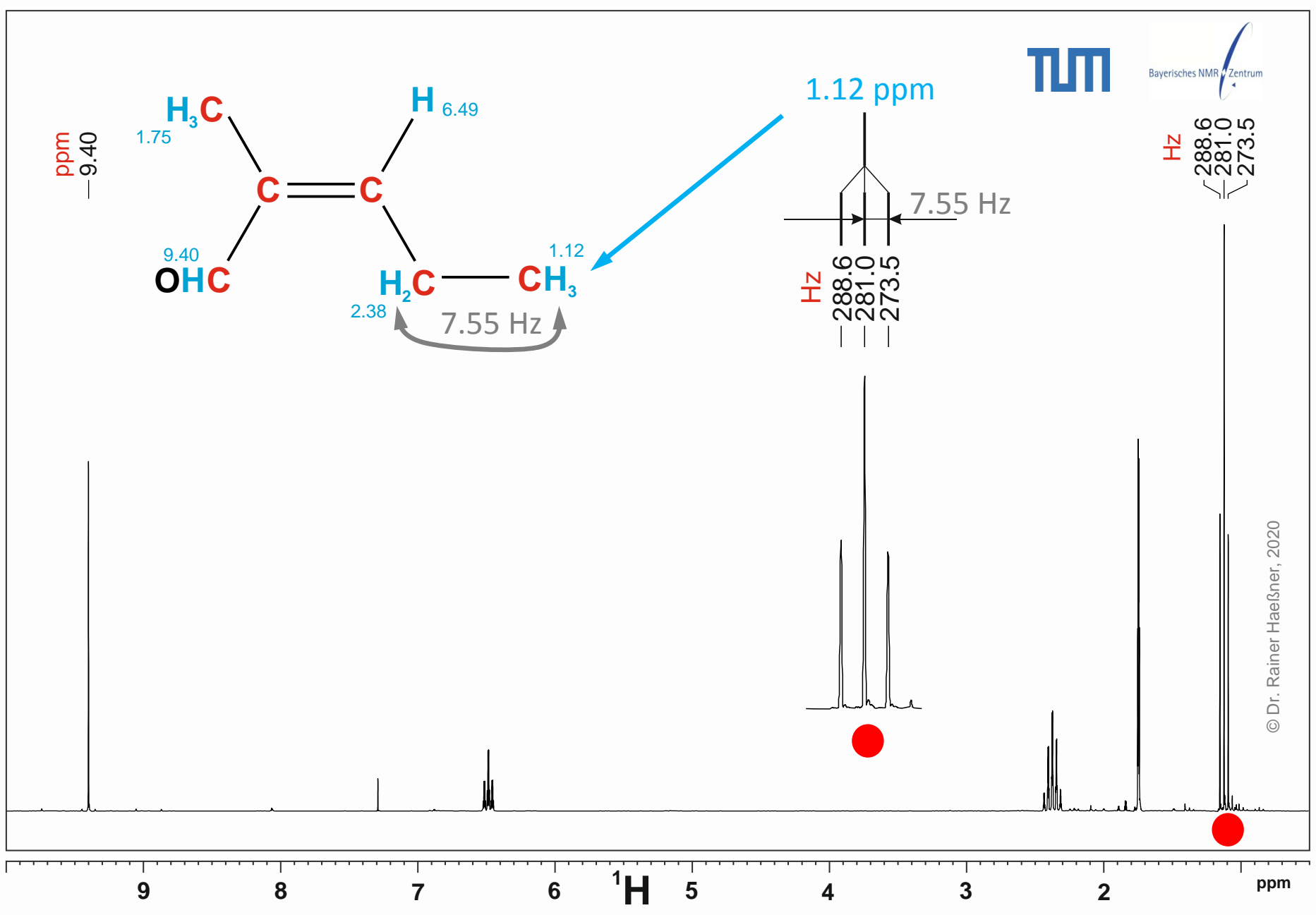
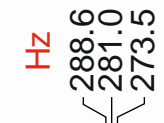
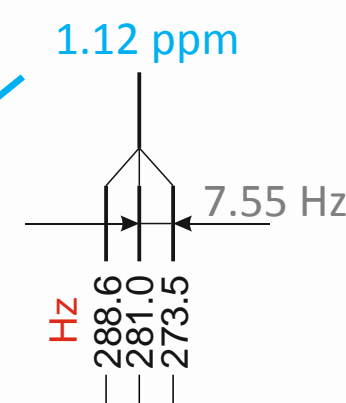
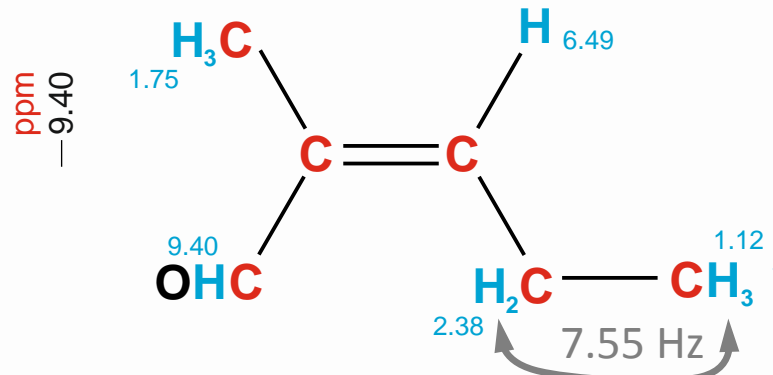
No other choice

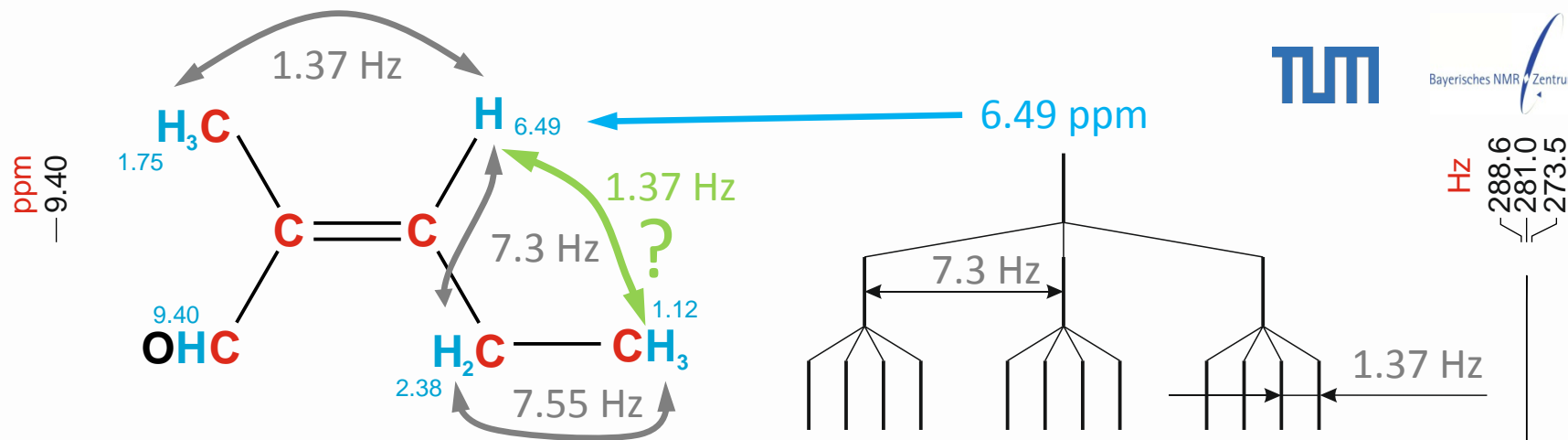


And this cross peak?

Four bond correlation across the double bond

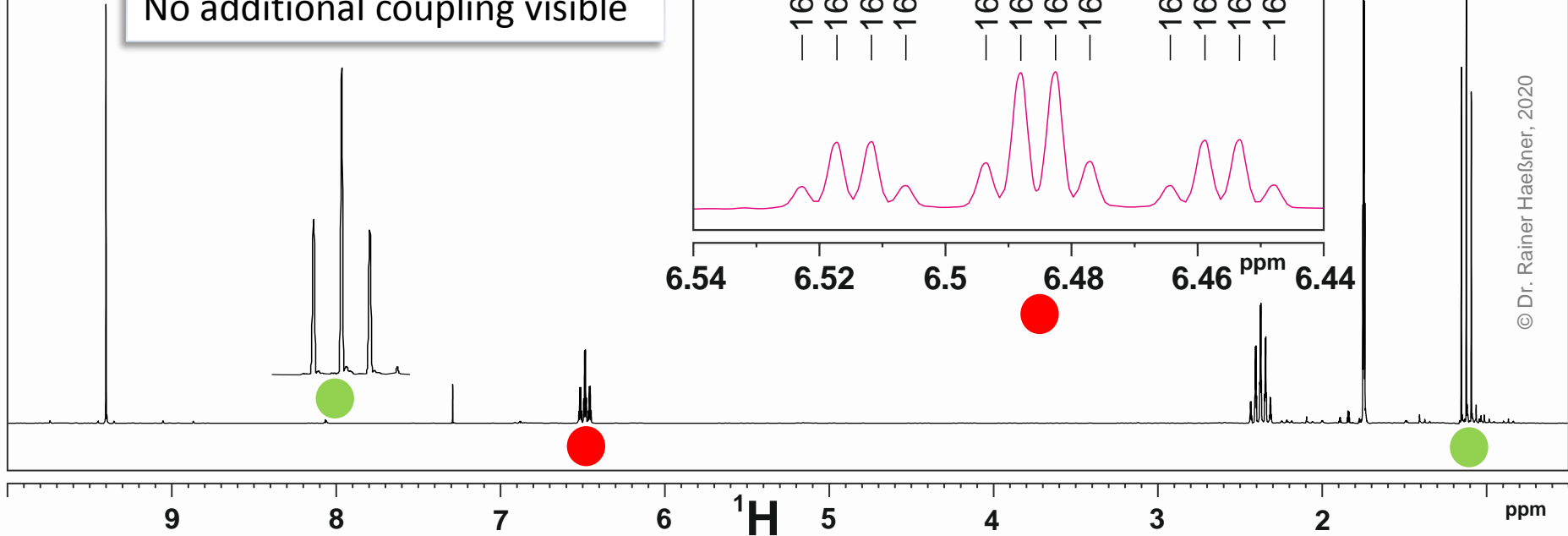
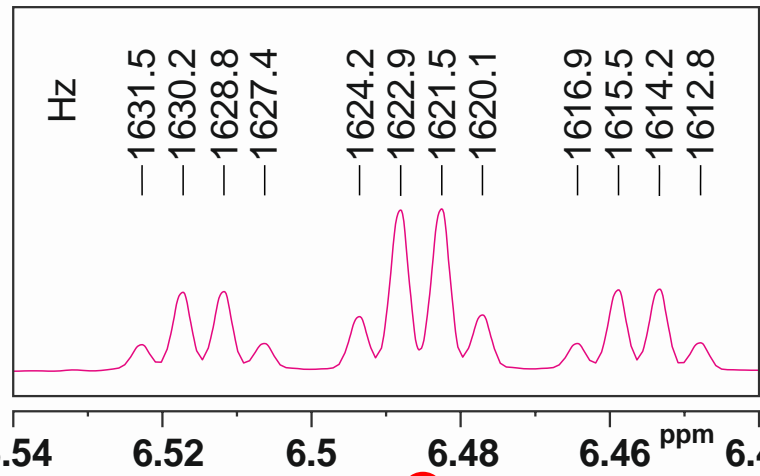


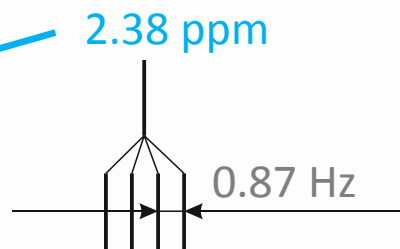
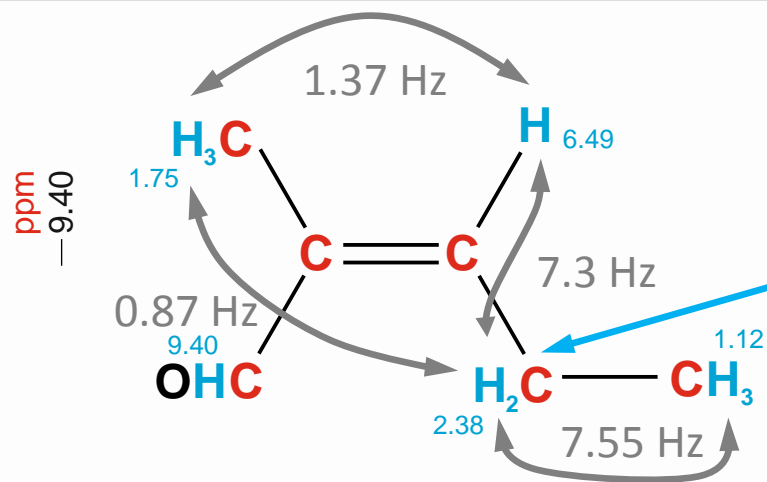




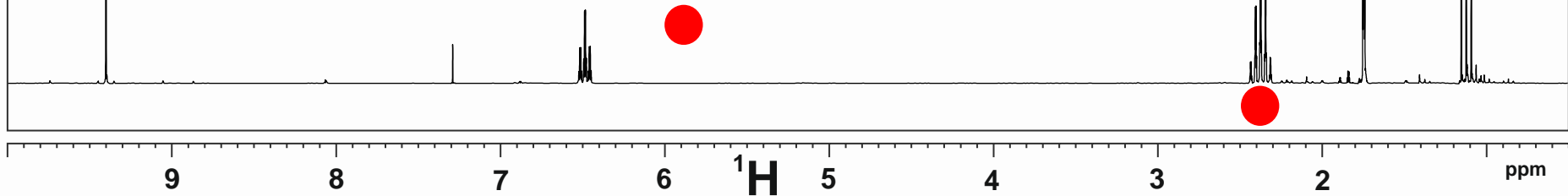
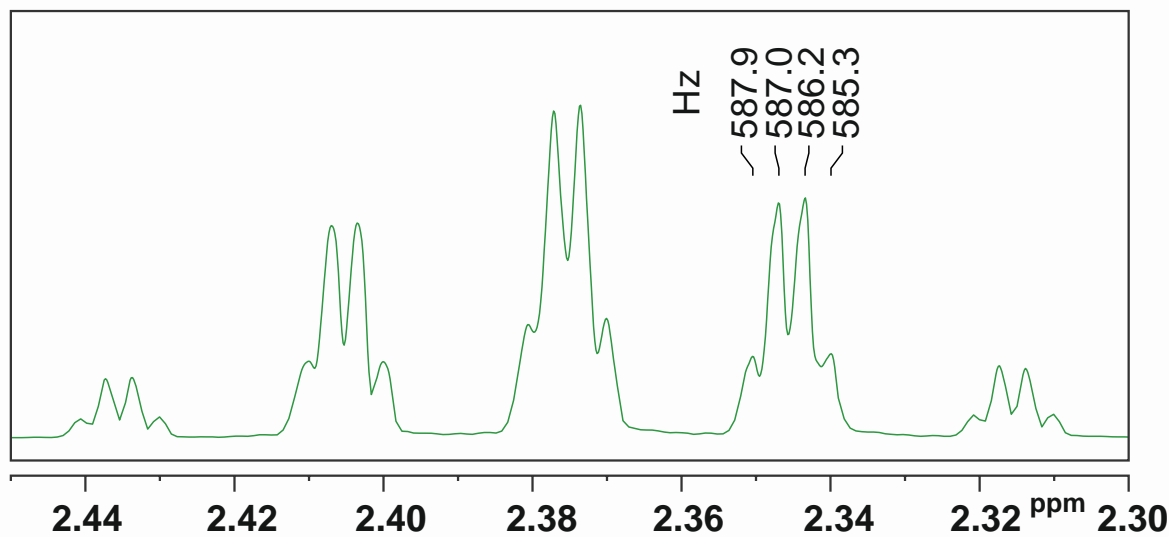
Why not?

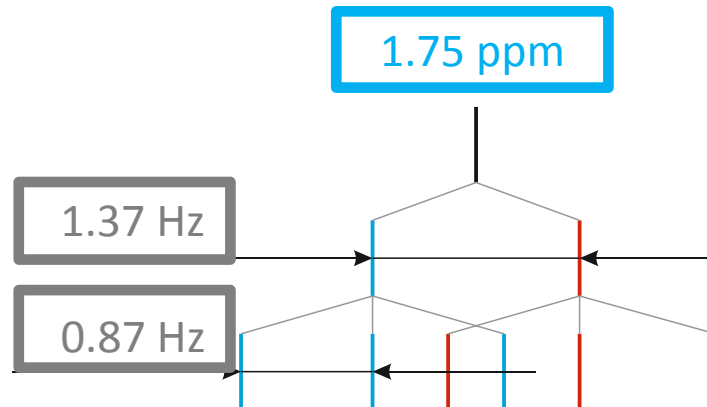
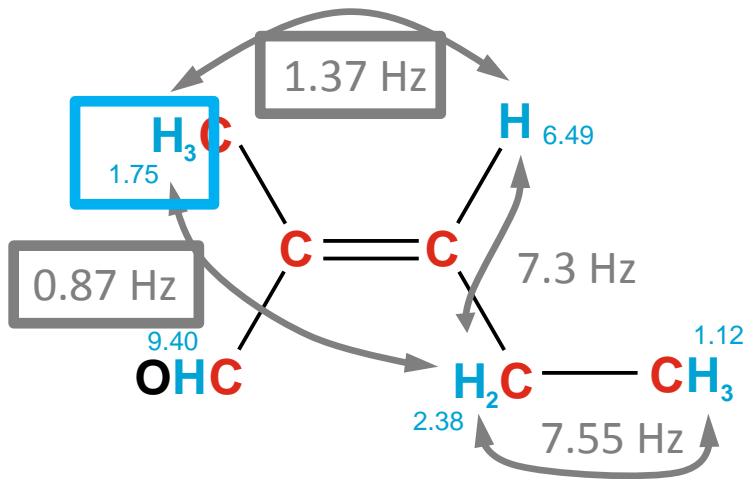
No additional coupling visible





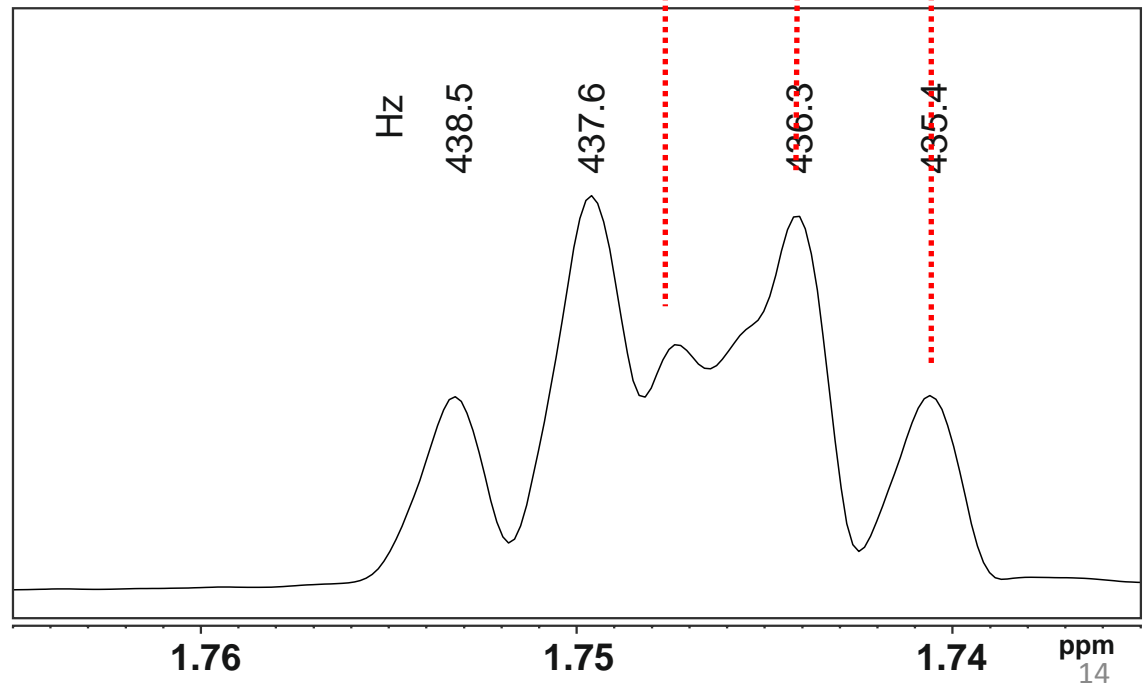
Hz  
 288.6  
 281.0  
 273.5

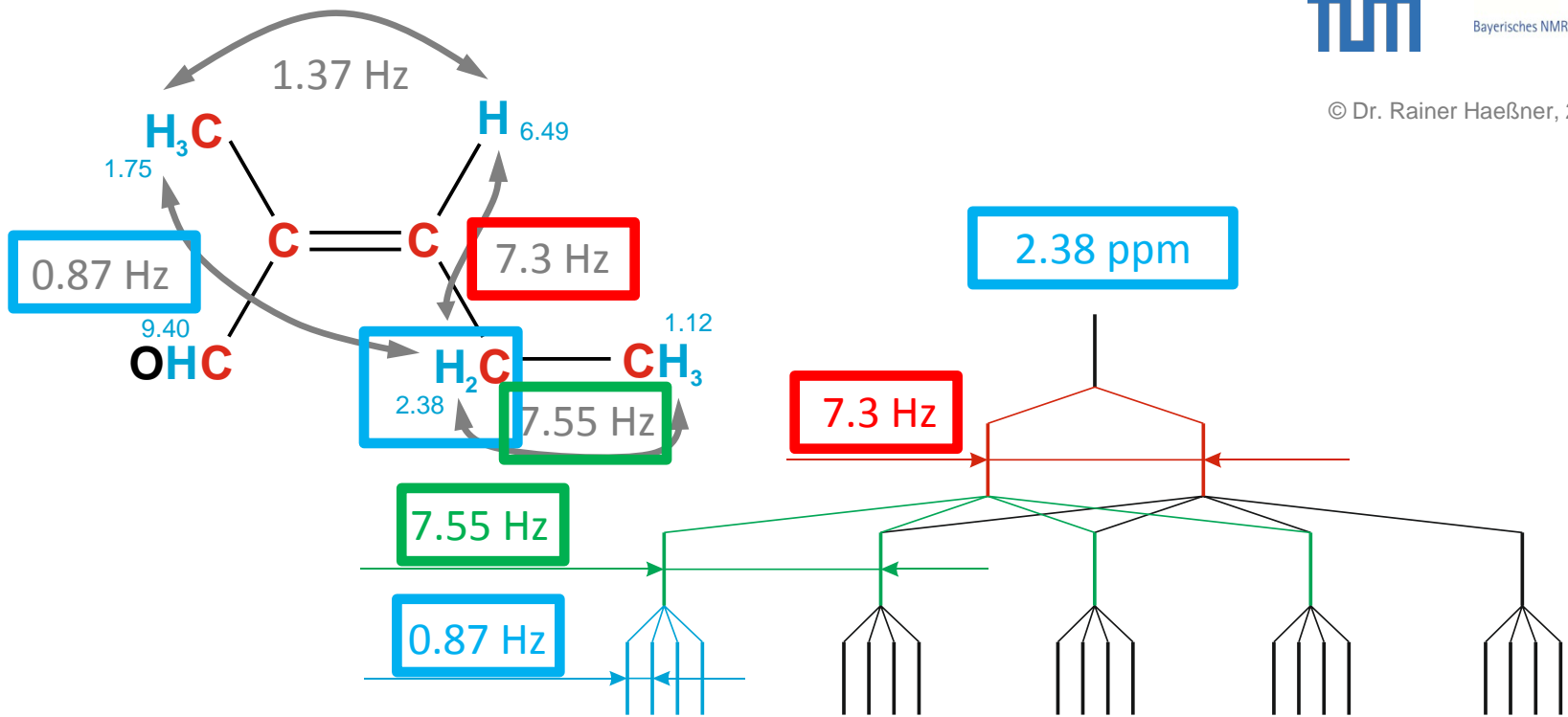




We have all coupling constants now

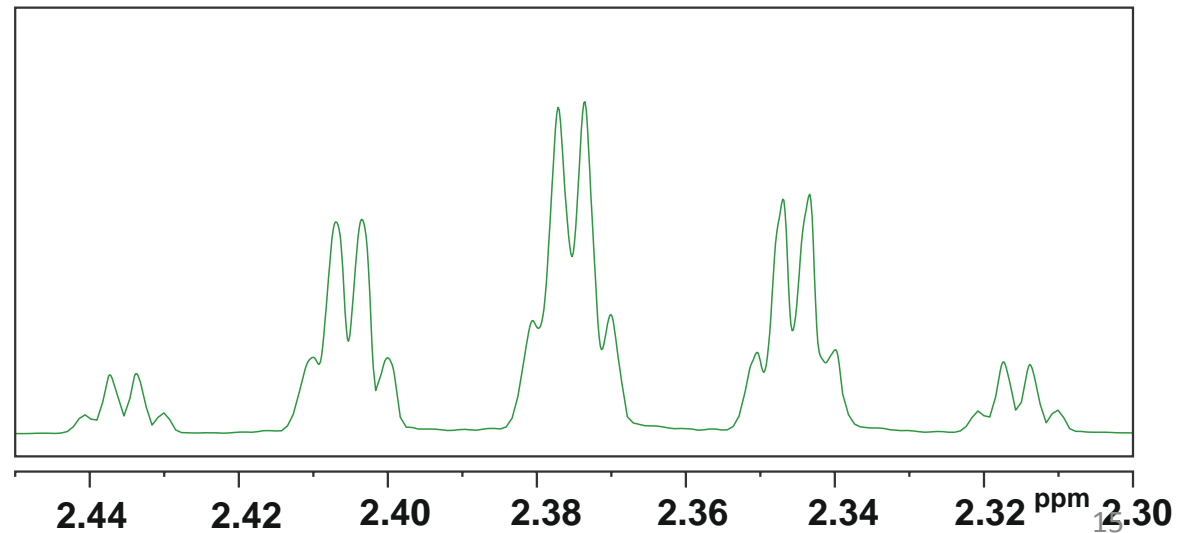
Lets predict the pattern of one slightly more complex signal





**That's no quartett of quintetts!**

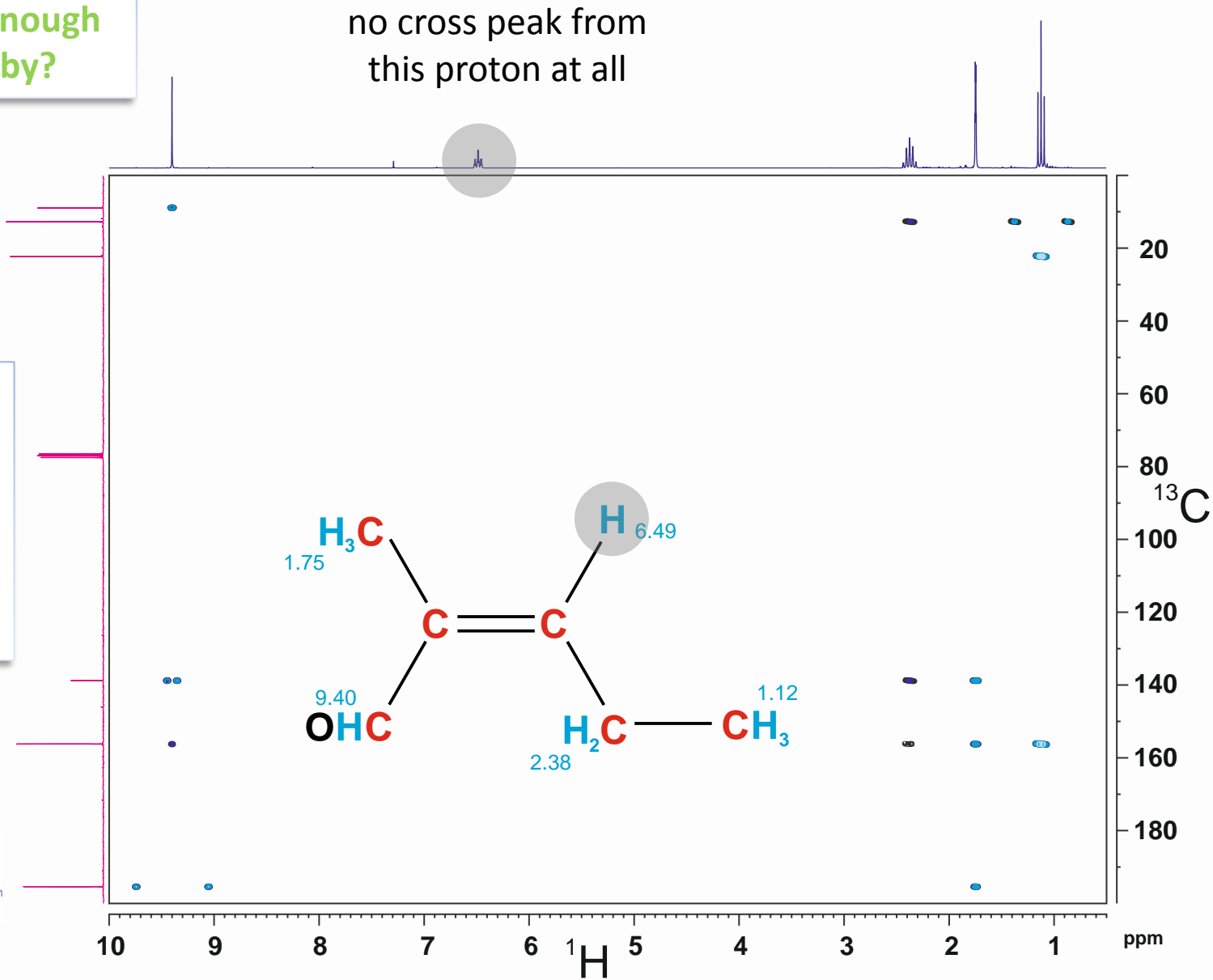
It only looks like that simple, because 7.3 Hz and 7.55 Hz are nearly identical.



Why is there no cross peak, although enough carbons are nearby?

no cross peak from this proton at all

For a detailed explanation please crawl for evolution time and transfer function!





There is another one bond correlation. Have a look around!

