

# Patterns of student reasoning while interpreting organic chemical spectra

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**NDSU**

CHEMISTRY AND BIOCHEMISTRY

What is problem solving?

# Problem Solving

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“Problem solving is what chemists do, regardless of whether they work in the area of synthesis, spectroscopy, theory, analysis, or the characterization of compounds”  
(Bodner & Herron, 2002)

# Problem Solving in Chemistry

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General chemistry problems:

- Stoichiometry
- Equilibrium

Organic chemistry problems:

- Synthesis

...Spectroscopy?

See: Camacho, M., and Good, R. (1989). Problem solving and chemical equilibrium: Successful versus unsuccessful performance. *Journal of Research in Science Teaching*, 26(3), 251-272.

Cartrette, D.P., and Bodner, G.M. (2010). Non-mathematical problem solving in organic chemistry. *Journal of Research in Science Teaching* 47, 643-660.

Herron J. D. and Greenbowe T. J. (1986). What can we do about Sue: A case study of competence, *Journal of Chemical Education*, 63, 526-531.

Kozma, R.B., and Russell, J. (1997). Multimedia and understanding: Expert and novice responses to different representations of chemical phenomena. *Journal of Research in Science Teaching*, 34(9), 949-968.

# Research Questions

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What is the nature of student reasoning while solving structures of organic compounds?

What is the diversity of the structures students produce?

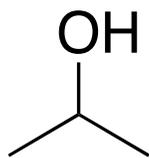
# Methodology

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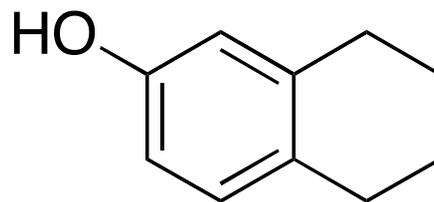
Interviewed 20 students

Two institutions

Solved from  $^1\text{H}$  NMR spectra for:



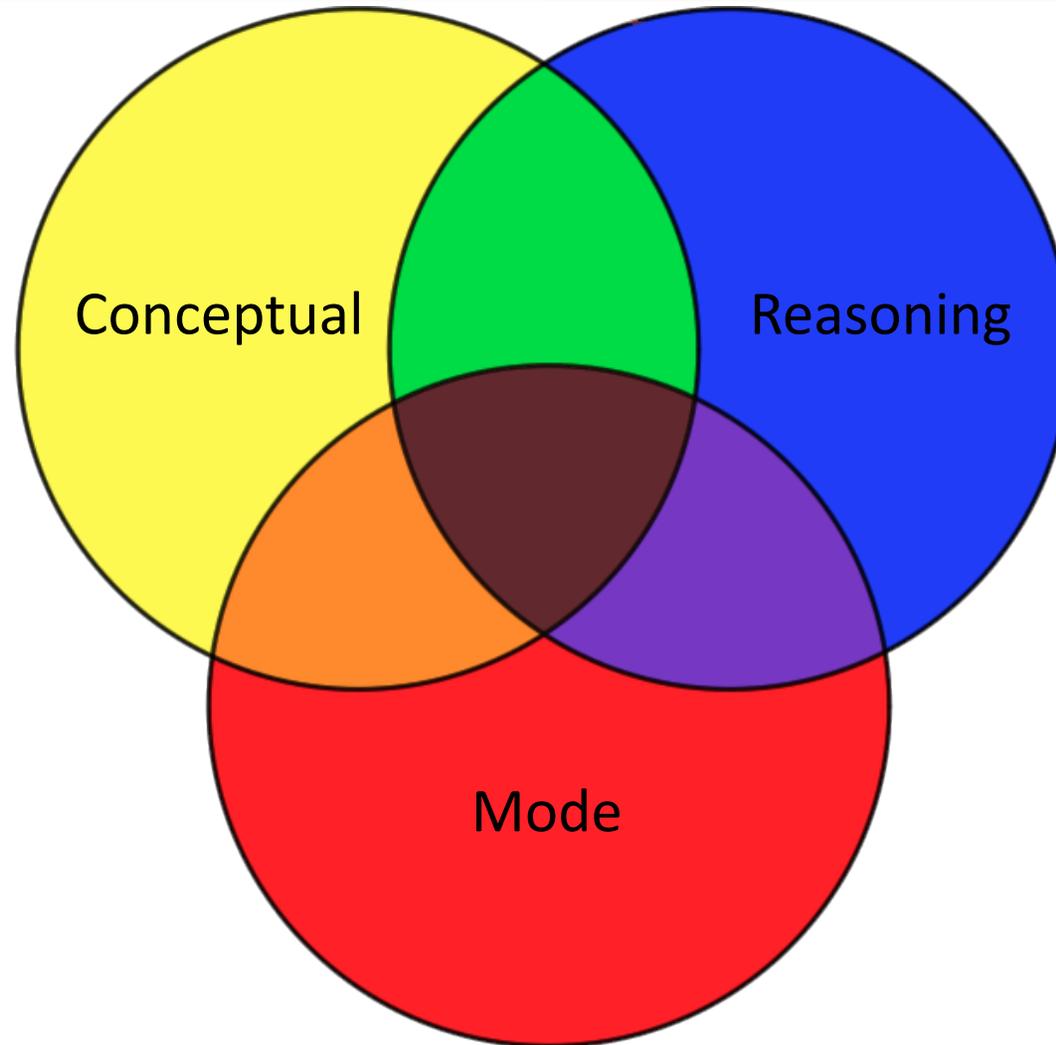
and



Adapted Schönborn and Anderson's 3P-SIT protocol...

# Model of factors that determine students' ability to interpret ERs<sup>2</sup>

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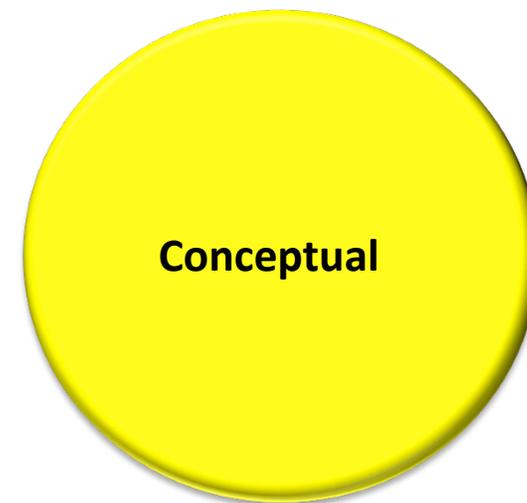
# An Adapted 3P-SIT—Phase 1

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What do you know about organic spectroscopy and  $^1\text{H}$  NMR?

Characterizes understanding of main principles of  $^1\text{H}$  NMR:

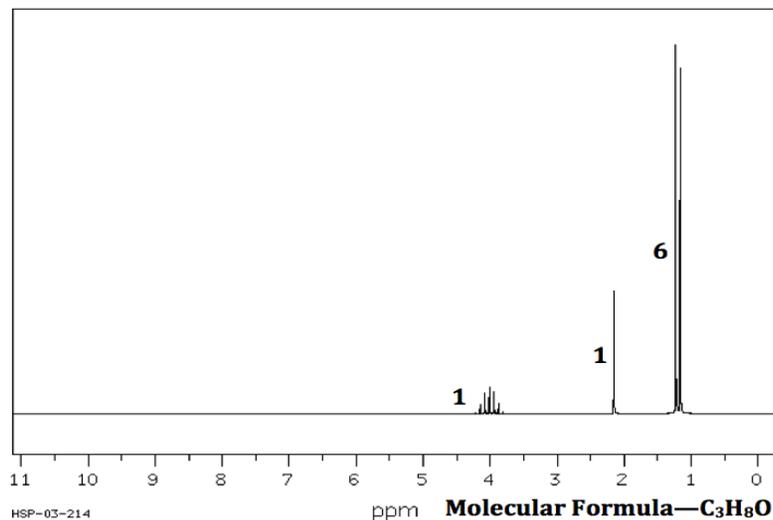
- Number of signals
- Chemical shift
- Splitting
- Integration



# An Adapted 3P-SIT—Phase 2A

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What is the structure of this compound?



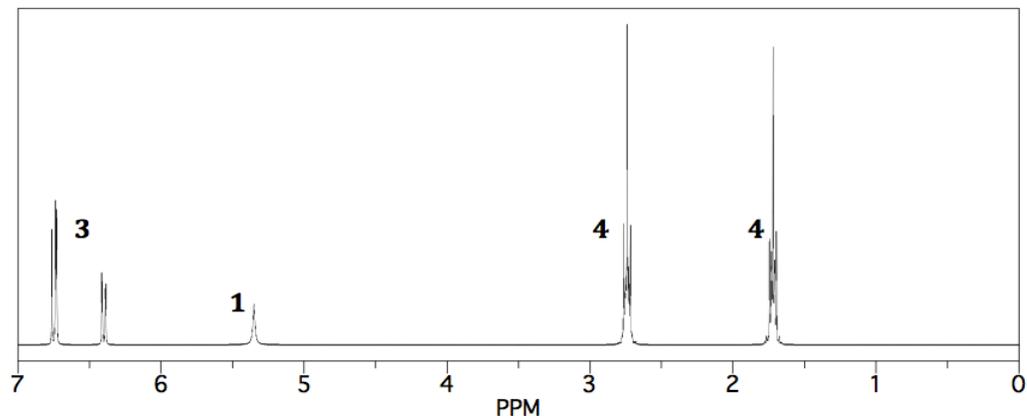
Primes interviewee and establishes a baseline of their solving ability.

**Reasoning**

# An Adapted 3P-SIT—Phase 2B

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What structure is represented here?



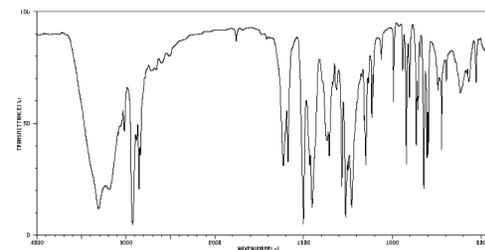
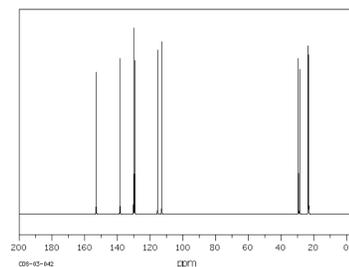
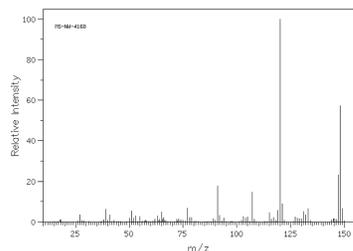
Molecular Formula— $C_{10}H_{12}O$

Reveals how students reason with the  $^1H$  NMR spectrum and what concepts they draw on while solving.

Reasoning

# An Adapted 3P-SIT—Phase 3

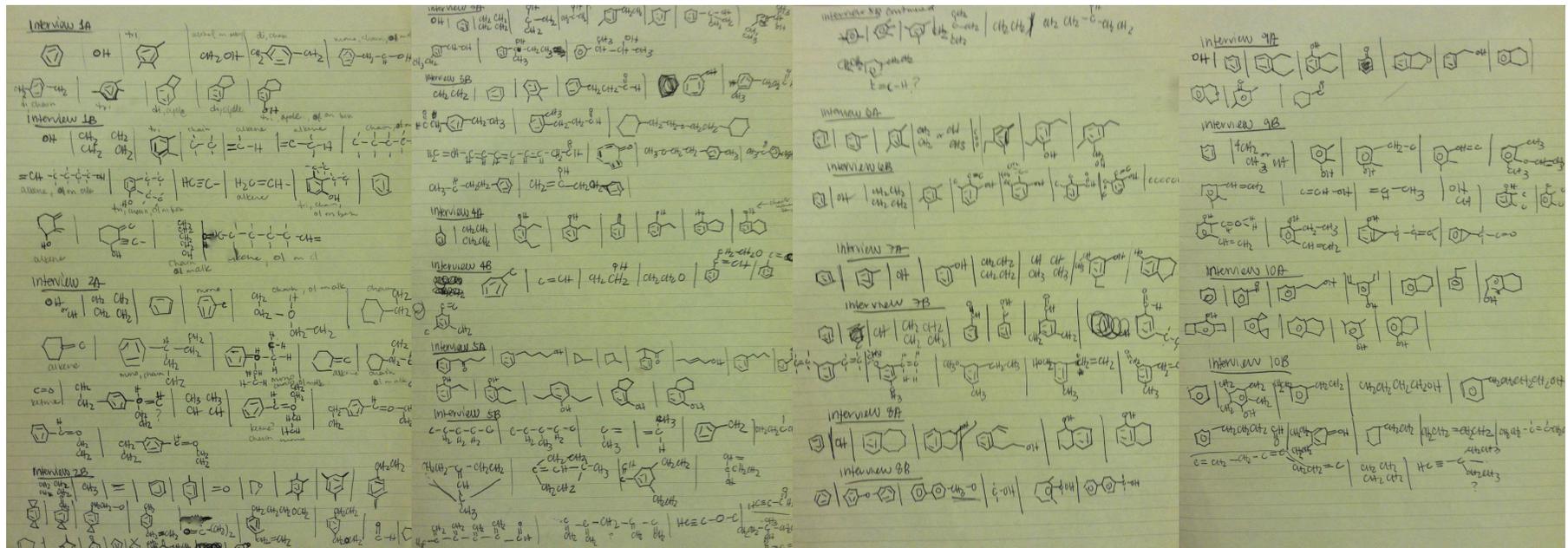
What about the spectrum itself was confusing?  
Could additional spectra help you?



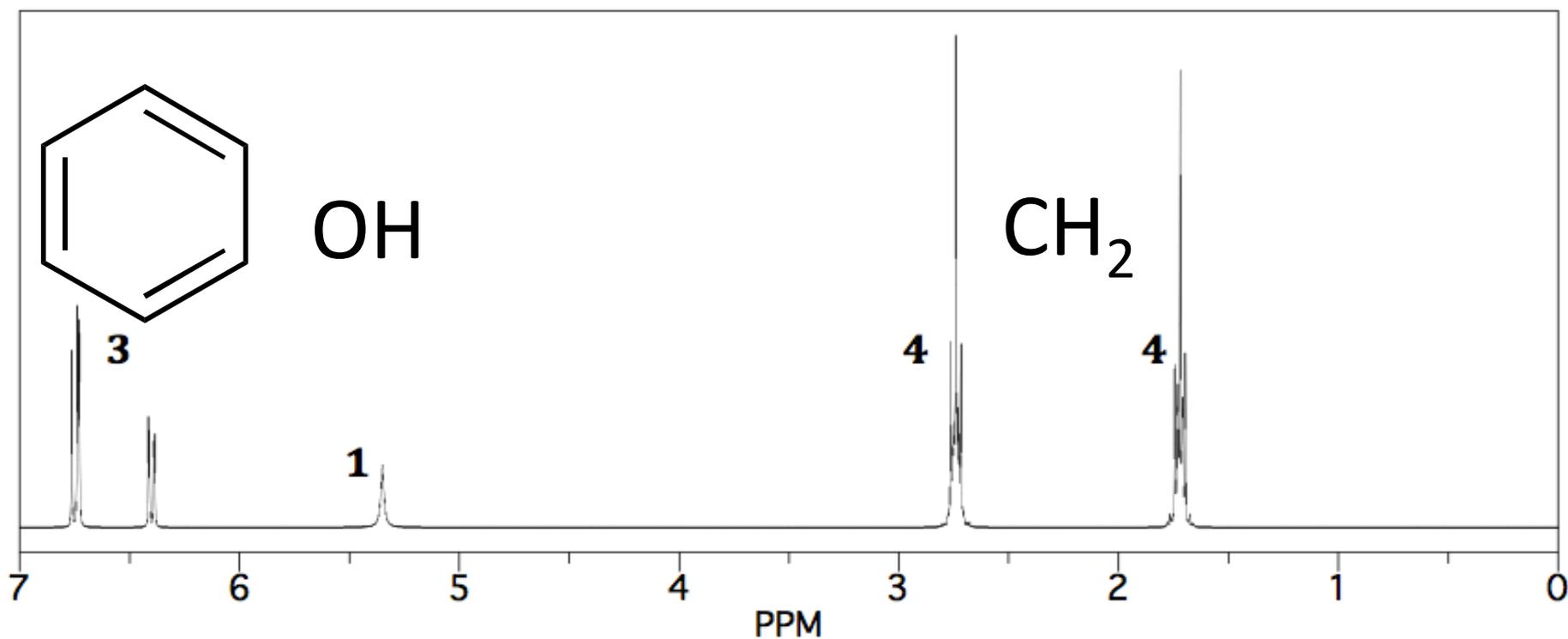
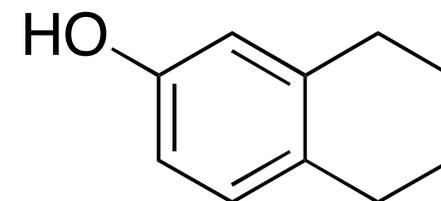
Probes mode and introduces  
additional spectra to uncover  
reasoning independent of mode.

**Mode**

# What did we get?



# Pieces of the Puzzle

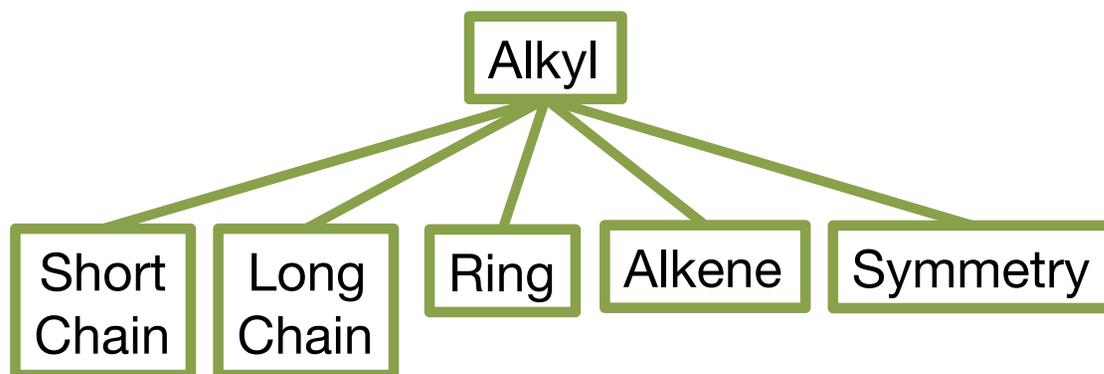
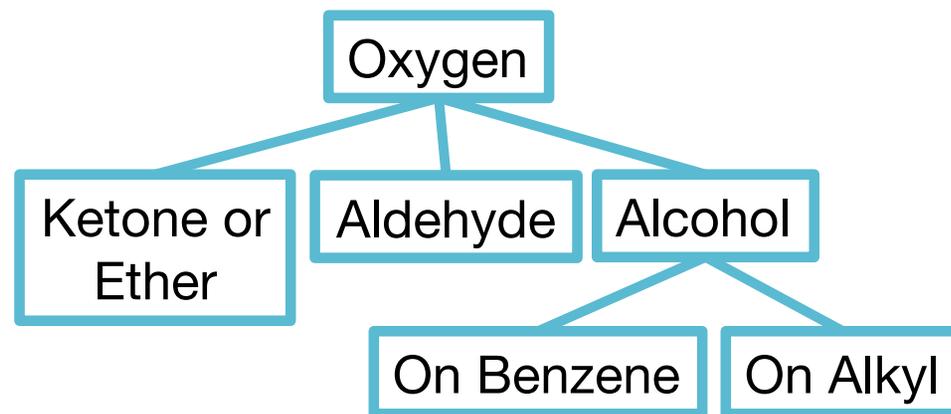
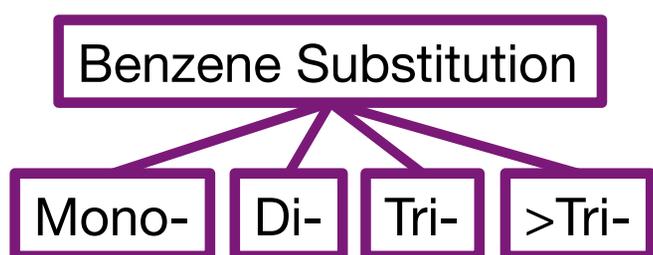


**Molecular Formula—C<sub>10</sub>H<sub>12</sub>O**

What happens when they put it all together?

# Diversity of student generated structures

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# Benzene Substitution

Benzene Substitution

Mono-

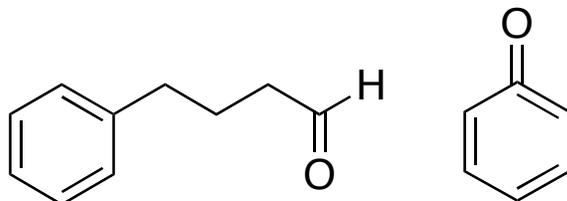
Di-

Tri-

>Tri-

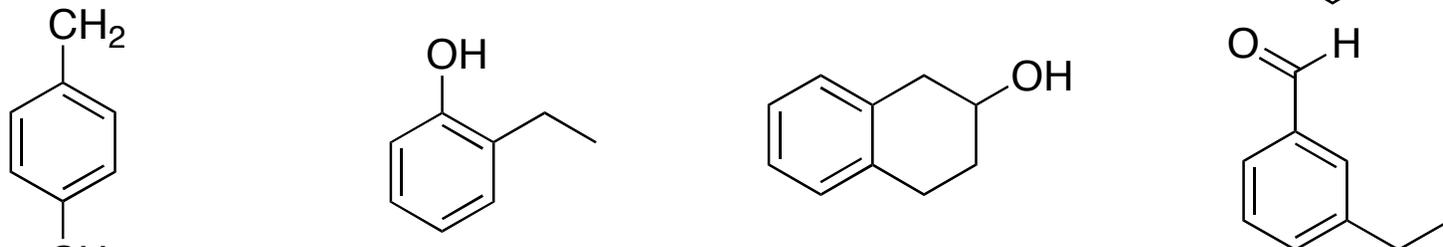
Mono-

75%



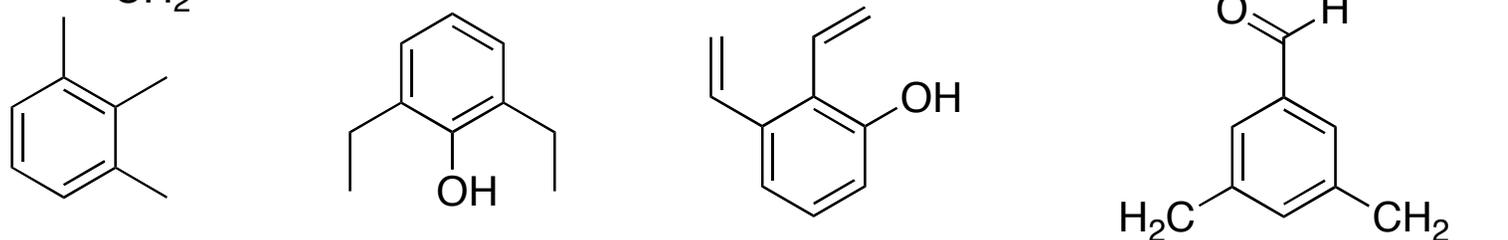
Di-

75%



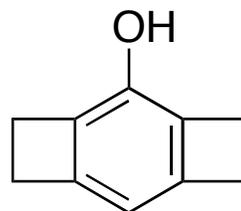
Tri-

90%



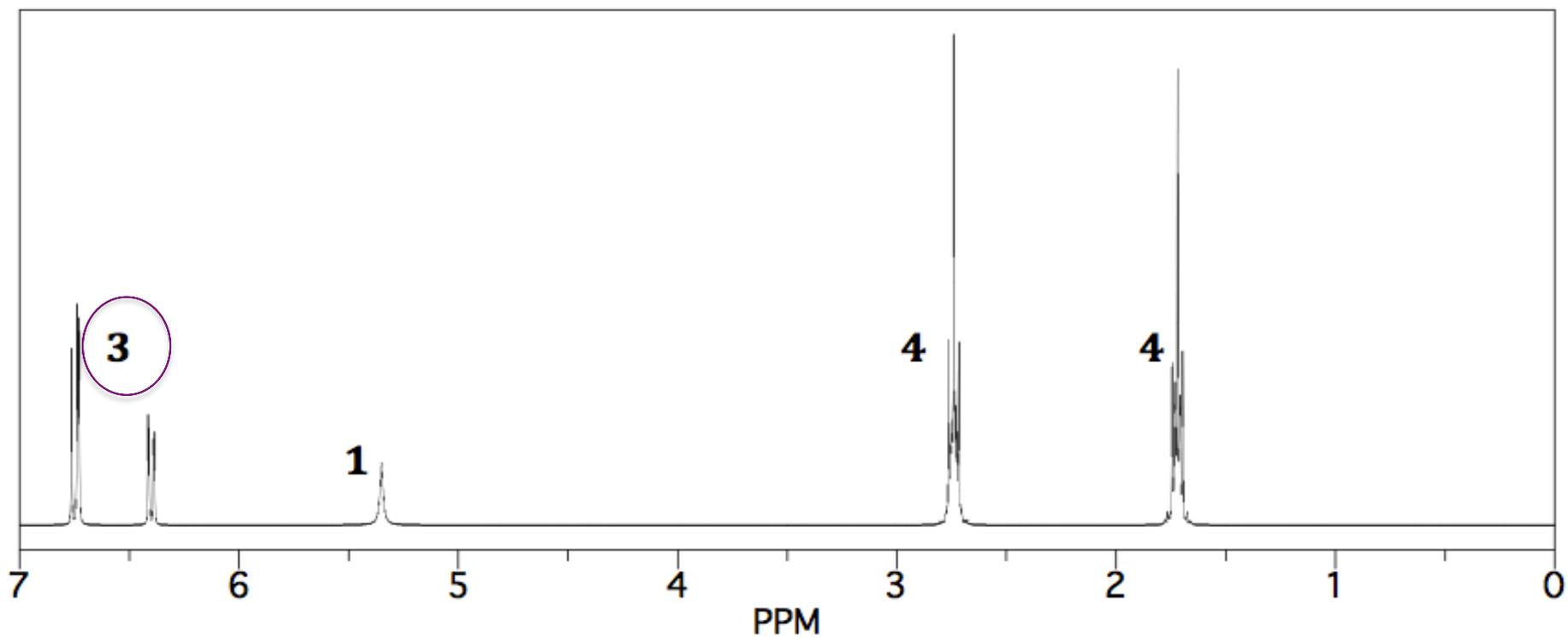
...or More

20%



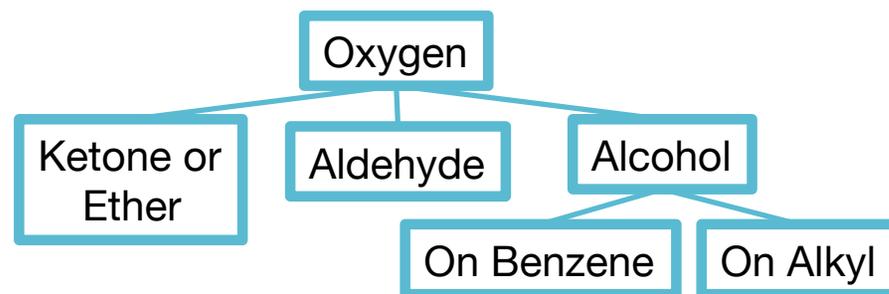
# Benzene Substitution

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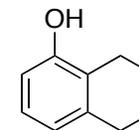
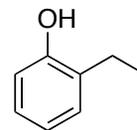
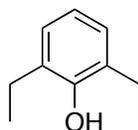


**Molecular Formula— $\text{C}_{10}\text{H}_{12}\text{O}$**

# Oxygen

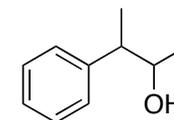
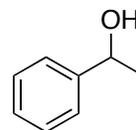
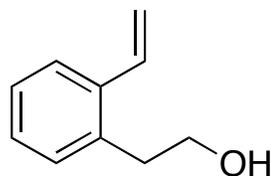


Benzyl alcohol



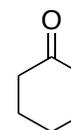
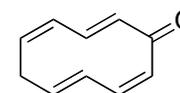
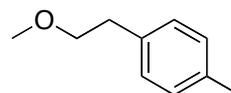
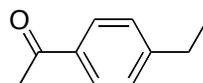
60%

Alkyl alcohol



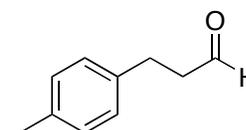
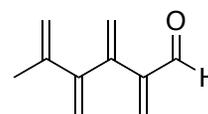
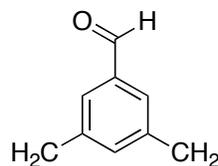
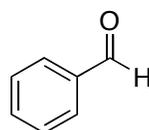
65%

Ketone or ether



60%

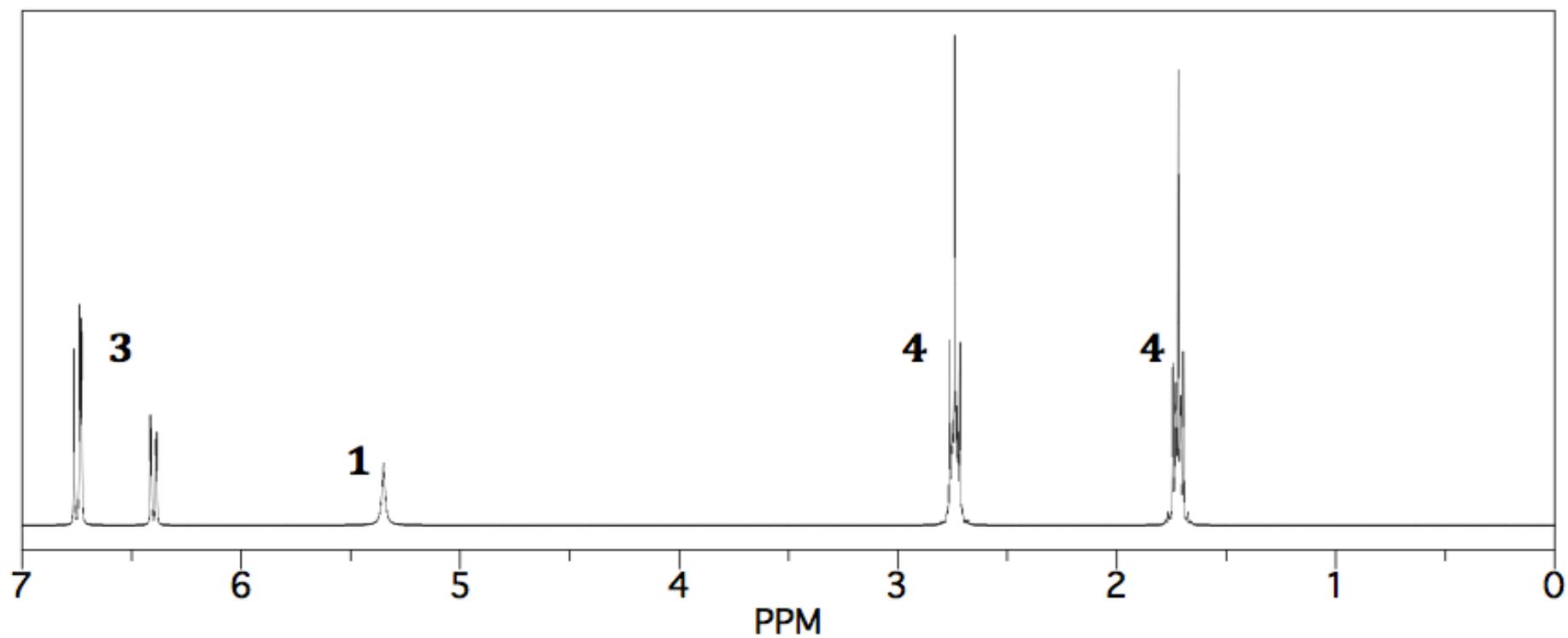
Aldehyde



40%

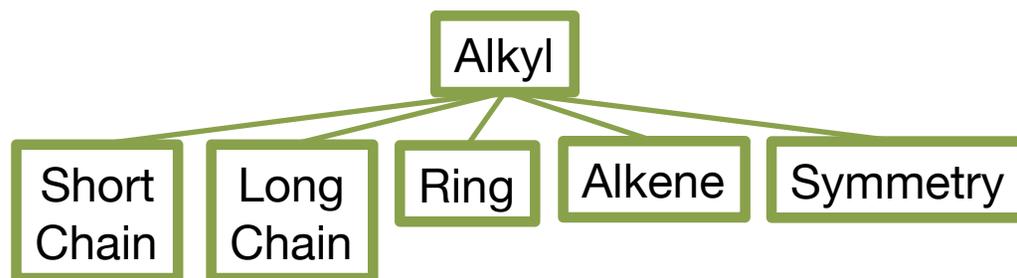
# Oxygen

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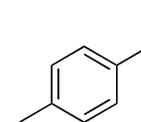
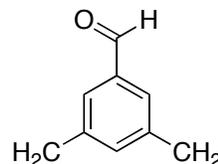
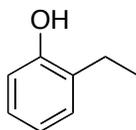
**Molecular Formula— $\text{C}_{10}\text{H}_{12}\text{O}$**

# Alkyl



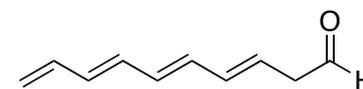
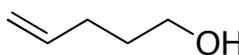
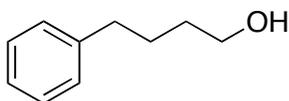
## Short chain

100%



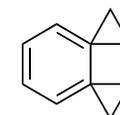
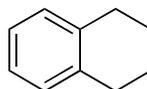
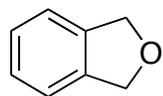
## Long chain

50%



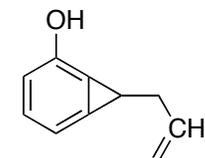
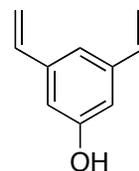
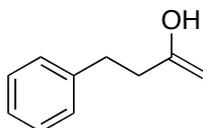
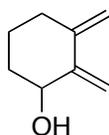
## Ring

55%



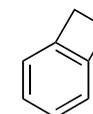
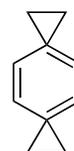
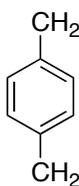
## Alkene

60%



## Symmetry

95%



# Implications/Future Work

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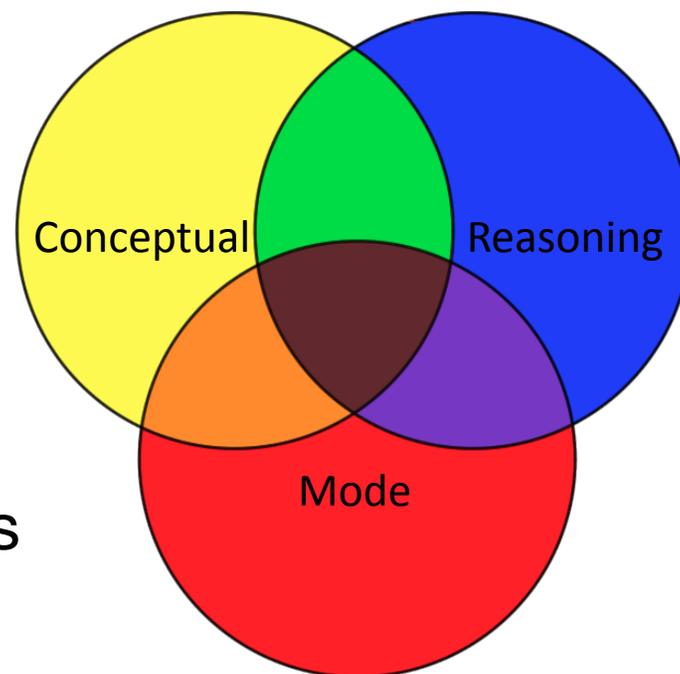
What are students reasoning with?

Is there a part of the spectrum that they are focusing on... or not focusing on?

Are the structures they draw based on structures they've seen before?

What triggers a student's progression from one structure to the next?

How do they reason with the principles of NMR?



# Acknowledgements

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Dr. Erika Offerdahl

Dr. Gregory Cook

Dr. Jennifer Momsen

Dr. Mukund Sibi



NDSU STEM Ed Colleagues

NDSU Department of Chemistry and  
Biochemistry