

Introduction to 1H-NMR Spectroscopy Hydrogen NMR interpretation is more complex than 13C-NMR, but provides extra information that is unavailable from carbon NMR. In interpreting carbon NMR, we focused on how many unique carbon lines were present, and where they were located (chemical shifts). In hydrogen NMR, but two additional factors, “integration” and “splitting”, are useful.

The four facets of 1H NMR spectroscopy:

1. Number of signal sets \Rightarrow the number of symmetry-unique hydrogens
2. Chemical shifts \Rightarrow chemical environment/hybridization/functional groups
3. Integration \Rightarrow how many hydrogen atoms cause a signal.
 - 3H \Rightarrow CH₃ group (or 2H and 1H groups superimposed)
 - 2H \Rightarrow CH₂ group (or two nonequivalent 1H groups superimposed)
 - 1H \Rightarrow CH or OH group
4. Splitting \Rightarrow information about how many H's are connected to adjacent carbons
 - N lines \Rightarrow N-1 “neighbor” H's (when working from spectrum to structure)
 - N neighbors \Rightarrow N+1 lines (when you know what a structure is, and you're trying to predict what it's spectrum should look like)

Summary of Steps in 1H NMR Interpretation: (Not all will be needed to get the Answers Today)

1. Count how many signal sets you have. **This will tell you how many types of hydrogen-bearing carbons** you have.
 - Hydrogens attached to symmetry-equivalent carbons will give equivalent signals
2. **Check diagnostic “chemical shift” windows** of the lines **to provide yes-or-no answers regarding the presence or absence of key functional groups** in your molecule.
3. Check the integration of each signal set.
 - 3H \Rightarrow CH₃ group 2H \Rightarrow CH₂ group 1H \Rightarrow CH or OH group
4. Check the splitting of each signal set.
 - For a signal set with N lines \Rightarrow N-1 hydrogens will be attached to carbons directly connected to the carbon of the signal set

I. Number of Signal Sets

1. Nonequivalent H's have different chemical environments and give different signals
2. Symmetry-equivalent H's have the same chemical environment and give the same signal
 - The number of signal sets tells you how many different types of hydrogens are present
3. On an **achiral** molecule (alkenes excepted), hydrogens on a given carbon will be equivalent.
 - all three H's on a CH₃ group
 - both H's on a CH₂ group
4. The number of signal sets may sometimes differ from the number of carbons:
 - a. Symmetry equivalent carbons and hydrogens
 - b. Hydrogen-free Carbons: No attached H, no H signal! (Carbonyl carbons rarely have H's...)
 - c. OH Groups: OH as well as CH's give hydrogen signals
 - d. CH₂ H's are NONEQUIVALENT in “Cis/Trans” Situations:
 - In **Alkenes**, or when there is a **chiral center** in the molecule.
5. Strategy Keys:
 - a. If possible, determine how many signal sets you have in a spectrum. (Useful when working from spectrum to structure).
 - b. For a particular structure, determine how many signal sets you should have. (Useful when matching unknown candidate structures with actual spectra, as in today's lab.)

- c. **End-Check:** Check that the number of signal sets in your spectrum matches with the structure you believe you actually have! If not, structure needs correction!
- d. **Beware of overlaps!**

II. “Chemical Shifts” of the Signal Sets

7's (6.5-8.4)	Aromatic sp^2 hybridized C-H's
3's (2.8-4.5)	Oxygenated sp^3 hybridized C-H's (halogenated and nitrogenated alkyl C-H's will also come in this window, although no candidates for today's lab). Oxygenated sp^3 -carbons are routinely present for the following functional groups that contain oxygen single bonds: <ul style="list-style-type: none"> • alcohols, • ethers, or • esters
2's (1.8-3.1)	Allylic sp^3 hybridized C-H's (sp^3 hybridized C-H's that has a double bond attached to the sp^3 hybridized C). Allylic signals routinely appear when one of the following double-bonded functional groups is present: <ul style="list-style-type: none"> • carbonyls, (ketones, esters, aldehydes, acids, amides) • alkenes, or • aromatics
1's (0.7-2.0)	sp^3 hybridized C-H's, with no attached Functional Groups <ul style="list-style-type: none"> • Note: Many molecules with non-functional alkyl portions will give a lot of signal in this area.
0-5 (anywhere!) (normally 1.5-3.5 range)	Alcohol O-H hydrogens

How do I process and use what I see from my Chemical Shifts?

- 1. Recognize OH's.** Because an OH can come anywhere, it can easily cause mistaken conclusions. An OH in the 2's, for example, can falsely make you think that you have an allylic C-H when you really don't. Thus it is really helpful to recognize OH's when they appear so that they don't confuse you. **Three recognition factors for OH signals:**
 1. They always **integrate for 1H**, never for 2H or 3H
 2. They usually **appear as singlets**. The only way to have a 1H singlet is for it to be an OH.
 3. If you have an alcohol OH signal, of course you will also have some C-H signals in the 3.0-4.5 area. (For the hydrogens on the hydroxy-bearing carbon.)
- 2. Check each of the zones. Each one gives you a yes or no answer about the presence of absence of the featured group.**
 - Do I have something in the 7's? (Other than a solvent singlet...)? If yes \Rightarrow aromatic
 - Do I have something in the 3's? If yes \Rightarrow alcohol, ether, or ester (or OH)
 - Do I have something in the 2's? If yes \Rightarrow ketone, aromatic, or alkene (or OH)
 - Do I have something in the 1's? If yes \Rightarrow some nonfunctional alkyl carbons (or OH)

3. End-Check: Check that the functional groups indicated by your chemical shift information match with the structure you believe you actually have! If not, structure needs correction!

Miscellaneous Chemical Shifts Notes

1. Approximate 1's, 2's, 3's, and 7's and spillover: The regions are somewhat approximate, and have some spillover. But it's still useful to basically talk about the "1's", "2's", "3's", etc. to discuss the major windows. Even though something might actually come at 4.2, it's still useful to refer to that as appearing in the "3's" group and make conclusions accordingly. I'll still refer to something as coming in the "1's" group even if it comes at 0.8.
2. Hybridization: sp^2 hybridized C-H's come above 5, sp^3 hybridized C-H's come below
3. Oxygenated C-H's come higher than non-oxygenated analogs.
4. When two functional groups are impacting, chemical shifts change. (If a CH₂ group is doubly allylic, it won't show in the 2's. If a CH₂ is doubly oxygenated, it won't show in the 3's.)
 - For this introductory lab, you won't need to worry about this.
5. OH's are wildcards because they can come anywhere, and can cause confusion.

III. Integration Unlike in carbon NMR, the sizes of H-NMR signal sets are very useful and informative.

1. The signal area ("integral") is proportional to the number of hydrogens causing the signal.

$CH_3 \Rightarrow 3H$	$CH_2 \Rightarrow 2H$	$CH \text{ or } OH \Rightarrow 1H$
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2. The key is not the signal height, but rather the signal **area**.
 - The signal **area** is measured by "integration lines". Differentiate integration marks, and what they mean, from signal lines themselves.
3. Relative areas correlate ratios of H's. **Convert to simple whole-number ratios** (and round off freely).

$1:1 \Rightarrow CH_2 \text{ to } CH_2, \text{ or } CH_3 \text{ to } CH_3$	$1.5:1 \Rightarrow 3H:2H \text{ (} CH_3 \text{ to } CH_2)$
$2:1 \Rightarrow 2H:1H \text{ (} CH_2 \text{ to } OH)$	$5:2 \Rightarrow 5H:2H \text{ (} C_6H_5 \text{ to } CH_2, \text{ common with aromatics)}$
$3:1 \Rightarrow 3H:1H \text{ (} CH_3 \text{ to } OH)$	$6:1 \Rightarrow \text{Common with isopropyls, } CH(CH_3)_2$
4. Clean sets involving equivalent H's give clean, symmetric signal sets:
 - a. $1H \Rightarrow CH \text{ or } OH$
 - b. $2H \Rightarrow CH_2$
 - c. $3H \Rightarrow CH_3$
 - d. $6H \Rightarrow 2 \text{ equivalent } CH_3 \text{ groups}$
5. Unsymmetrical messy sets involving overlapping signal sets. (these will routinely not look nice and symmetric...)
 - a. $3H \Rightarrow OH \text{ overlapping a } CH_2$
 - b. $4H \Rightarrow \text{two overlapping but not exactly equivalent } CH_2 \text{ groups; or a } CH_3 \text{ overlapping an } OH \text{ or } CH$
 - c. $5H \Rightarrow \text{common in the } 7's, \text{ for } 5 \text{ overlapping arene } H's; \text{ also common in the } 1's, \text{ when a } CH_3 \text{ and } CH_2 \text{ overlap}$

How do I process and use what I see from my Integrations?

1. Distinguish "Clean" Signal Sets from Overlapping Signal Sets
 - o Clean ones look symmetric, overlapping sets do not
2. **For the Clean sets, the integration tells you what kind of group you have**
 - a. $1H \Rightarrow CH \text{ or } OH$ (methine or hydroxyl group)
 - b. $2H \Rightarrow CH_2$ (methylene group)
 - c. $3H \Rightarrow CH_3$ (methyl group)
 - d. $6H \Rightarrow 2 \text{ equivalent } CH_3 \text{ groups}$
3. **End-Check: Check that the "groups" your integration shows match with the structure you believe you actually have! If not, your structure needs to be corrected!**

IV. Splitting Hydrogen signals are routinely split into multiple lines. The number of lines in a signal set tell us nothing about “the signal” C-H’s themselves that cause the signal (whether it’s a CH₃ or CH₂ group, or whether it’s allylic or oxygenated...). But the splitting tells us something else that is really useful: what kind of CH groups are attached to the group of interest! It provides great information about “neighbor groups” and helps explain how the components of an organic molecule are sequenced.

Rules of “Splitting”

- **N-1 Rule:** N lines \Rightarrow N-1 neighbor H’s (H’s directly attached to carbons attached to the signal C-H group causing the signal)
 - The N-1 Rule is useful when working from spectrum to actual structure
 - **N+1 Rule:** N neighbor H’s \Rightarrow N+1 lines
 - The N+1 Rule is useful when working from structure to actual spectrum
1. OH hydrogens don’t participate in splitting ~75% of the time. About 25% of time they do.
 2. C-H hydrogens participate in splitting (always)
 3. For today’s labs and for simple molecules, the N-1/N+1 rules are good. The rules actually work only if the neighbor H’s are equivalent. The rule can break down when some of the neighbor H’s differ significantly from each other
 4. Splitting from H’s further distant than neighbor carbons sometimes occurs, but usually the amount of splitting is too small to worry about
 5. Physics Origin: hydrogens are quantized little magnets. Neighbor hydrogen magnets can align so as to either reinforce (spin up) or counteract (spin down) the external magnetic field

N+1 Rule (Given structure, how many lines a spectrum should give)										
Neighbors	2	3+2	2	0	Neighbors	0	-	2	2+3	2
Lines	3	6	3	1	Lines	1	-	3	6	3
(Notice: OH doesn't split...)										
N-1 Rule (Given spectrum, how many neighbors a structure should have)										
	Lines	1 (s)inglet				Lines	2 (d)oublet			
	Neighbors	0				Neighbors	1			
	Lines	3 (t)riplet				Lines	4 (q)uartet			
	Neighbors	2				Neighbors	3			etc.

6. Splitting nicknames:
 - 1 line \Rightarrow singlet (s) 2 lines \Rightarrow doublet (d) 3 lines \Rightarrow triplet (t)
 - 4 lines \Rightarrow quartet (q) 5 lines \Rightarrow pentet (p) >5 lines \Rightarrow multiplet (m)

How do I process and use what I see from my Splitting?

1. Use **integration** for a given signal to determine if your signal set is a CH₃, CH₂, or CH group
2. Then use the number of lines in the signal set and the N-1 Rule to see how many hydrogens must be present on neighboring carbons that are attached to your signal set
3. **End-Check:** Check that the structure you believe you actually have would give the splitting you are actually seeing in your spectrum. If not, your structure needs to be corrected!

V. Standard Summary Report and/or Prediction Formats There is a standard summary report format for H-NMR's which addresses chemical shift, integration, splitting, and the source hydrogens.

Ex: $\text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (I'll number the carbons from left to right...)

Summary Report Format

Shift	Int	#lines(split)	Source
3.79	2H	3 (t)	(CH2-2)
3.48	3H	1 (s)	(CH3-1)
2.34	2H	3 (t)	(CH2-4)
2.16	3H	1 (s)	(CH2-6)
1.55	2H	5 (p)	(CH2-3)

Prediction Format

Source	Shift	Int	#lines(split)
(CH3-1)	3's	3H	1 (s)
(CH2-2)	3's	2H	3 (t)
(CH2-3)	1's	2H	5 (p)
(CH2-4)	2's	2H	3 (t)
(CH2-6)	2's	3H	1 (s)

VI. Miscellaneous

- Subtracting the Solvent Lines: Don't Count the Singlet at 7.26** CDCl_3 is routinely used as solvent, but is contaminated by trace CHCl_3 which gives a signal at 7.26.
- Subtracting the Reference Line: Don't Count the Line at 0** A reference chemical $[(\text{CH}_3)_4\text{Si}]$ is included to define where "zero" is.
- Subtracting the Water Line:** Often a little moisture will be in the solution. This will often appear somewhere around 1.6, but it wanders depending on hydrogen-bonding factors.
- Subtracting the Acetone Line?** Acetone shows a singlet at around 2.15. If acetone has been used to rinse but hasn't dried yet, this will appear. But it normally integrates incorrectly.
- How do I know what's a real signal versus a signal arising from an impurity that I should ignore?** For today, if in doubt ask the instructor! The instructor will confirm which lines you should or shouldn't consider in doing your analysis. However, one useful recognition tip is that if something integrates badly, it's likely a contaminant. Integrals are supposed to be nice whole-number ratios (1:1, 2:1, 3:2, etc.)
- Beware of Overlapping.** Overlapping is most routine in the benzene area (7's), and also in the alkyl area (1's), but happens elsewhere as well. OH signals often overlap other signals. For this week, if in doubt ask.

Summary of $^1\text{H-NMR}$ Interpretation

I. Number of Signal Sets

II. “Chemical Shifts” of the Signal Sets

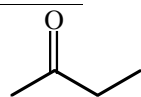
7's (6.5-8.4)	<u>Aromatic</u> sp^2 hybridized C-H's
3's (2.8-4.5)	<u>Oxygenated</u> sp^3 hybridized C-H's. Oxygenated sp^3 -carbons are routinely present for the following functional groups that contain oxygen single bonds: <ul style="list-style-type: none"> • <u>alcohols</u>, • <u>ethers</u>, or • <u>esters</u>
2's (1.8-3.1)	<u>Allylic</u> sp^3 hybridized C-H's (sp^3 hybridized C-H's that has a double bond attached to the sp^3 hybridized C). Allylic signals routinely appear when one of the following double-bonded functional groups is present: <ul style="list-style-type: none"> • <u>carbonyls</u>, (ketones, esters, aldehydes, acids, amides) • <u>alkenes</u>, or • <u>aromatics</u>
1's (0.7-2.0)	sp^3 hybridized C-H's, with <u>no attached Functional Groups</u> <ul style="list-style-type: none"> • <u>Note:</u> Many molecules with non-functional alkyl portions will give a lot of signal in this area.
0-5 (anywhere!) (normally 1.5-3.5 range)	<u>Alcohol</u> O-H hydrogens

III. Integration These **must be simple whole-number ratios** (2:1, 3:1, 3:2, etc..)

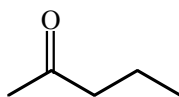
IV. Splitting

- **N-1 Rule:** **N lines** \Rightarrow **N-1 neighbor H's** (H's directly attached to carbons attached to the C-H group causing the signal)
 - The N-1 Rule is useful when working from spectrum to actual structure
- **N+1 Rule:** **N neighbor H's** \Rightarrow **N+1 lines**
 - The N+1 Rule is useful when working from structure to actual spectrum

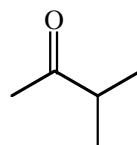
Note: OH hydrogens don't participate in splitting (normally)

Hydrogen NMR, The Experiment. What you need to do, an Overview.**H-NMR Unknown Candidates**

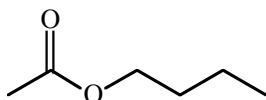
2-butanone



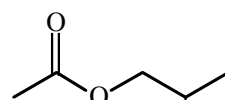
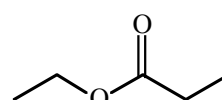
2-pentanone



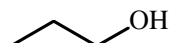
3-methyl-2-butanone



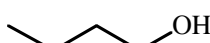
butyl ethanoate

2-methylpropyl
ethanoate

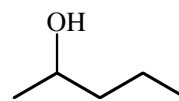
ethyl propanoate



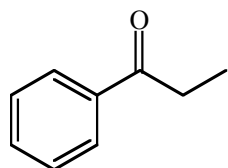
1-propanol



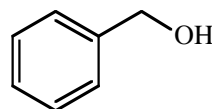
1-butanol



2-pentanol



propiophenone



benzyl alcohol

Lab and Lab Report Requirements**1. Prepare and run one sample.**

- Either use 1-2 drops, or more conveniently use a long pipet and load it up to maybe an inch (or less), and shoot that into your tube.
- Dilute with CDCl₃ solvent to 1/3 tube depth.
- The experiment run will be "Proton8"

2. Identify and interpret at least two NMR spectra.

- You can get the "other" NMR by opening somebody else's data from the queue or from the data folder.
- It may be your partner's data, but it doesn't need to be.
- There is a handin form later.

3. Get at least one full print for each of the two unknown

- Horizontal expansions are not required but may be very helpful to be able to see and interpret the splitting
- Manual integrations are not required but may be very helpful to recognize the integration values

4. Predict what some other structures would give. There is a handin form for this later.**5. Due date, 2010: Tuesday, 4:00. (Office gets locked at 4:30 normally, so get it in with some time to spare.)**

User's Guide to NMR: Compressed Version for Hydrogen NMR Organic Lab

- For help, see Dr. Jasperse, Hagen 407J, phone 477-2230
1. Prepare Sample
 - Proton NMR: 1 drop, dilute with CDCl₃ solvent to 1/3 tube depth.
 - Using a long pipet, fill it maybe 1 inch, shoot that into your tube, and dilute with CDCl₃.
 2. **Add sample to a Spinner/Turbine**
 3. **Adjust depth** by placing the turbine into the golden depth finder, and gently slide the sample till the tube just barely reaches the bottom
 4. **Load sample/turbine into autosampler.**
 - Note: DO NOT JUST GRAB OPEN THE AUTOSAMPLER DOOR WHILE IT IS LOCKED. YOU CAN DAMAGE THE ALIGNMENT BY FORCING IT OPEN WHEN IT IS LOCKED. IF THE STATUS LIGHT IS GREEN, YOU MAY NOT OPEN THE DOORS!
 - Press the round white **Access Request Button** on the panel below the sample trays/doors
 - **Wait until the "status" light turns to a solid yellow, and the message panel reads "door unlocked"**
 - Gently open the doors, and swap your sample/turbine(s) into the autosampler.
 - **Remember which site(s)** you placed it into!
 - Note: Samples can be added in this way to the autosampler even while the instrument is running somebody else's sample.
 - Note: The door needs to be closed when a sample is going to be ejected.
 5. **Login from within VNMRJ:** click **Unlock** (note: if VNMRJ is left open, as it should be for all of this week, then there will be a screensaver that goes black after a period of non-use. To get back in you will need to "unlock" the screen.)
 - User: nmr Password: none
 - Operator: Chem355 Password: nmr
 6. **Select/Prepare for the first experiment** (for the first experiment)
 - a. **New Study** (push button on lower left)
 - b. **Experiment Selection: Proton8** (on the left. The "UserStudies" folder at the lower left-hand corner of the Experiment Selector folders must be opened for this to be available.)
 - c. **Node/site identification.**
 - Click on the button showing where in the autosampler your sample is.
 - d. **Sample Name:** fill in your name
 - e. **Comment box:** fill in your name
 - f. **Shim:** this needs to be checked on (shimming takes extra time but is essential for good hydrogen spectra)
 7. **Submit** the experiment(s) by clicking the bright green **Submit** button on the lower left side.
 8. **Adding your Sample into the Sequence when the Autosampler is Already Running a Queue**
 - a. Prepare and correctly load your sample into the autosampler
 - b. At the computer, click on your sample node your, then:

- c. change the Sample Name: fill in your name
- d. change the comment name: fill in your name
- e. click submit.

9. Plotting an extra copies from the Queue

- a. Under **Study Queue** on the left, change the **View** to **Spectrometer** (you may need to click the “done” button first)
- b. A key will show up next to each completed node
- c. Click on your experiment.
- d. Below the viewscreen, click **Process** (3rd from left)
- e. Click **Plot** (2nd from bottom)
- f. Click **Automatic Plot Page** (top left)

10. Opening and Printing From the Data Folders

- a. Click on the Folder icon, upper left, the icon is right below the “Edit” menu.
- b. If you’re lucky, it will go directly to the home/nmr/vnmrsys/data/Chem355 folder.
- c. Double-click on the folder with your name.
- d. Double click on the file that has PROTON in it’s name
- e. Print as described in steps d-f above.
- f. To get the Folder icon to go back to the main Chem355 folder, click on the Folder icon again, then click ONCE only on the a little icon that shows an arrow up

11. Horizontal Expansions

- a. Make sure your spectrum is opened and displayed on the screen. If so, there should be a panel of display icons on the far right side.
- b. Click on the magnifying glass icon (6th icon down)
- c. Move your cursor to the left end of the zone you want to expand, then hold down the mouse button and slide it to the other end of the zone you want to expand.
- d. You can plot the expansion as described earlier (see 9)
- e. To return to the full display, you can either click on the 3rd icon or perhaps the 5th icon, and expand other zones as needed.

12. Defining Integrals: Manual Integration

- a. Make sure your spectrum is opened and displayed on the screen.
- b. Go to process (menu choice 3rd from left directly underneath the spectrum display)
- c. Choose “Integration” (6th menu item down)
- d. Hit “Clear Integrals” button
- e. Hit “Interactive Resets” button
- f. Then click on the left and right sides of a signal set to mark it for integration. Repeat this for each integration zone.
- g. To make the integral numbers easier, click Normalize Area to “Single Peak”
- h. Set the “integral area” to some nice number (1, 2, or 3, depending on whether you think you have a CH, CH₂, or CH₃)
- i. Click the “set integral value” button
- j. If your cursor was on the wrong integral or on no integral at all, click on an integral of choice and re-click the “set integral value” button again.
- k. You can plot as described earlier.

Hydrogen NMR Lab Handin**Name**

A. For each of the following chemicals, completely fill out the “Prediction Format” tables to predict what you would expect.

Standard Prediction Format: Ex: $\text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (Carbons numbered left to right...)

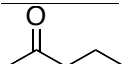
Source	Shift	Int	#lines(split)
(CH3-1)	3's	3H	1 (s)
(CH2-2)	3's	2H	3 (t)
(CH2-3)	1's	2H	5 (p)
(CH2-4)	2's	2H	3 (t)
(CH2-6)	2's	3H	1 (s)

Notes:

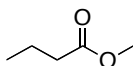
- Write numbers or letters next to each carbon in each structure to be used for identification purposes
- For the number of lines, you can include a number, you are not required to use the s, d, t, q descriptors
- For the chemical shifts for OH hydrogens, just write in “???”
- For OH hydrogens, assume they are 1line singlets and that they do not split CH hydrogens
- For the chemical shifts for others, enter either “1's”, “2's”, “3's”, or “7's”
- Aromatic hydrogens tend to overlap. For aromatic hydrogens, just combine them all. For example, write “aryl” for source; “7's” for chemical shift; “5H” for integration, and leave # lines empty.

StructurePredicted NMR

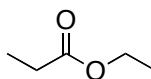
Source	Shift	Integ.	# lines

StructurePredicted NMR

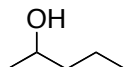
Source	Shift	Integ.	# lines



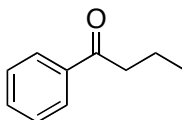
Source	Shift	Integ.	# lines



Source	Shift	Integ.	# lines



Source	Shift	Integ.	# lines



Source	Shift	Integ.	# lines

B. Draw the structures and use the Standard Summary Report format to interpret the features of the two unknowns, the NMR that you ran and the other NMR that you interpreted.

Example **Standard Summary Report:** $\text{CH}_3\text{OCH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (Numbered from left to right...)

Shift	Int	#lines(split)	Source
3.79	2H	3 (t)	(CH2-2)
3.48	3H	1 (s)	(CH3-1)
2.34	2H	3 (t)	(CH2-4)
2.16	3H	1 (s)	(CH2-6)
1.55	2H	5 (p)	(CH2-3)

1. Which unknown did you run yourself? (H1, H2, ...) _____
2. Draw its structure and make up numbers or letters next to each carbon.

Structure

Predicted NMR

Chemical Shift	Integ.	# lines	Source

3. If you know, which was the other NMR that you analyzed? (H1, H2, ...) _____
 - Note: you don't need to know or report this if you don't actually know, which is well possible...
4. Draw the chemical structure and make up numbers or letters next to each carbon.

Structure

Predicted NMR

Chemical Shift	Integ.	# lines	Source

C. Attach your NMR printouts. At minimum, include the unexpanded NMR printouts for both of the two samples. If you printed out horizontal expansions or printouts with manual integrations, you can include those too.