One and Two dimensional NMR Spectroscopy: Concepts and Spectral Analysis
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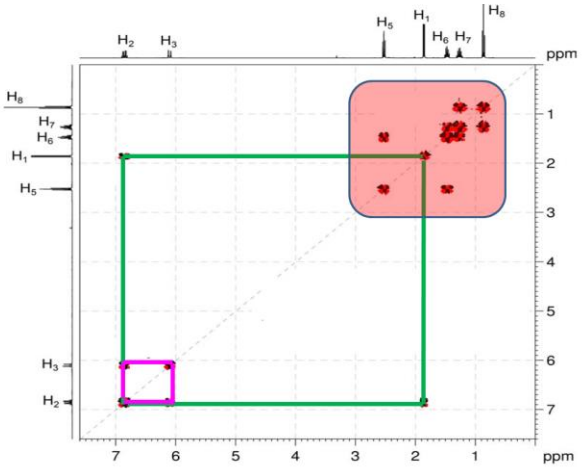
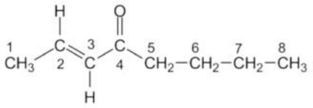
Lecture 56: Combined utility of COSY, TOCSY, HSQC, NOESY

Welcome all of you. In the last one or two classes we have been discussing about nuclear Overhauser effect spectroscopy. I introduced concepts, what is NOE, what are the factors that govern NOE and we discussed varieties of conditions, what will happen to the NOE whether there will be a gain or not at depending upon omega tau c. And we arrived at three conditions omega tau c greater than 1, omega tau c less than 1, omega tau c approximately equal to 1. And we said at omega tau c approximately equal to 1 NOE will be 0. In other two conditions, the extreme narrowing conditions and diffusion limits there will be NOE, positive or negative accordingly. So, we discussed a lot of the things about it. And also we arrived at the relaxation phenomena, in the sense dipolar relaxation which is responsible for this NOE, and where we are this fluctuating fields coming from? then we arrived at J(omega) and then the spectral density function depends upon the omega, of course, also probability on the transition probabilities, w1, w2 and w0. And then we also discussed about this fluctuating field coming because of the molecular motions, which depends upon tau c, the correlation time, and also on the larmor frequency, the spectrometer frequency. So, then varieties of factors are responsible for this, we discussed everything. And then at the end we arrived at the equations for NOE enhancement, and we saw NOE enhancement for a homonuclear spin in the extreme narrowing condition will be about half. That is what we saw in the case of homonuclear spins. For a heteronuclear case we also saw that depending upon the gyromagnetic ratios the enhancement factors will be different, and we we saw even up to 1200, 1500 times enhancement in some of the heteronuclei case, where proton is the irradiating spin. All these things we saw. And then we discussed varieties of possible NOE experiments, for example, steady state NOE where we are going to selectively irradiate a peak at a low RF power and then do another one with equal RF power at a far off place, far off resonance, and take the difference between two. And if there is any NOE enhancement for any of the particular spins which are close by, that gets reflected in the difference spectrum, that is a steady state NOE. We saw one or two examples of that. And also next is the transient NOE, that is a 2D NOE, we discussed a lot about 2D NOE, how you get the 2D NOE, everything. And then we discussed more about ROESY also. ROESY is the rotating frame Overhauser effect spectroscopy. That is done and favorablefor molecules, when the omega tau c is approximately equal to 1 where you do not get NOE, whereas ROESY always gives positive NOE. That is an advantage. So, we took one or two examples of ROESY and what are the complications involved in NOESY and

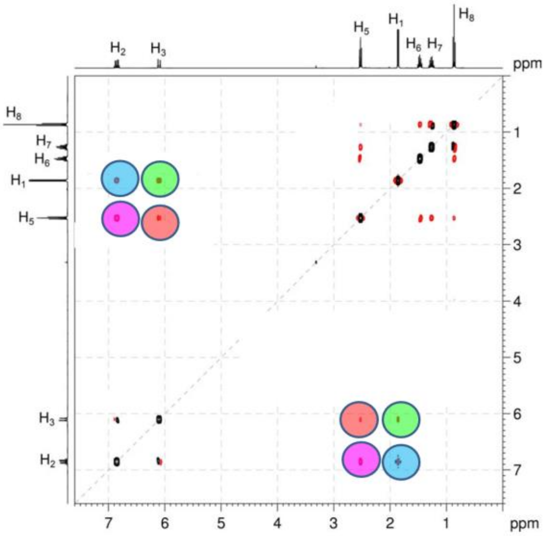
ROESY and all these techniques, including steady state NOE, what happens if you do not have a selective excitation where the frequency is not proper, what happens if the entire multiplicity region is not selectively saturated, the what will happen So, varieties of problems or complications are there. In all these experiments. some type of complications are there. And now we know how some of these can be overcome, that also we discussed. And then coming to 2D NOE we discussed the pulse sequence, and I told you we are going to get cross peaks which are symmetric with respect to the diagonal, we discussed that. And then we started even getting into the application of that to find out how NOESY can be used on some simple molecules. And we took one example to see how this NOESY helps in getting the conformation of that molecule. With that we will continue further today, we will take few more examples of NOESY, and how 2D NOE can be utilized to get the structure of or conformation of the molecules, some of the molecules. Some simple to complex molecules I will show, that is the important because, basically in this course I wanted to tell you about how we can analyze the spectrum, how we can use the different NMR techniques 1D and 2D, to get the structural information of your molecule.

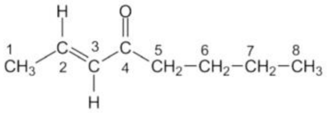
We will start with another molecule today. We did cis-pentene in yesterday, in the last class. Now we will start with another molecule, her,\e, this is the molecule, some name for it, trans-2-octen-4-one in DMSO-d6 in DMSO. This is a NMR spectrum. This is a COSY spectrum.





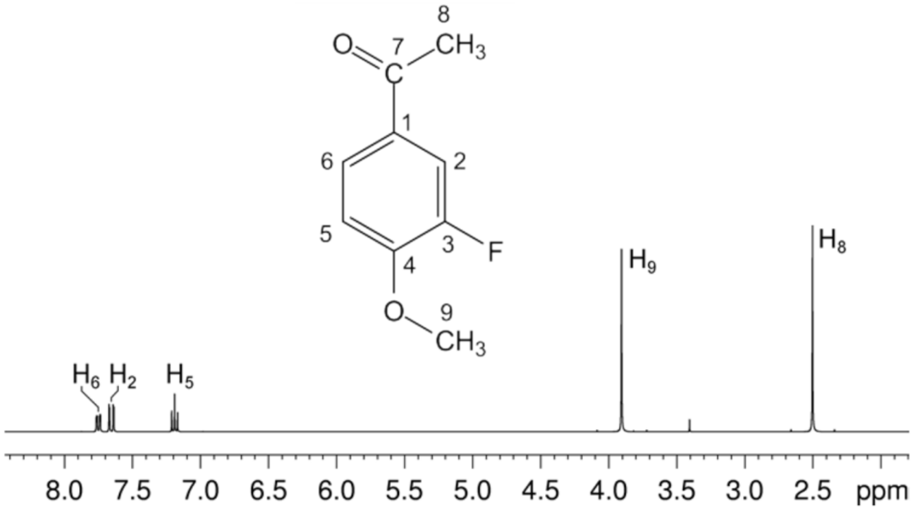
Of course very easily you can interpret the COSY spectrum. You can always star with CH3, I to always tell you, see proton H8 is there, it is triplet because of this and then this will be triplet of triplet because of this, and this will be triplet because of this, and very easily you can interpret it, but anyway COSY is going to help you in identifying all the peaks. Start with that one, here we have taken H2 proton, H2 is then which is correlated to H3 here, because this is an isolated pair, isolated spin system. You can see that, and there is lot separation, but CO is in between. And there is no coupling between this and this, so they are all forming isolated system, 1 2 and 3 are isolated spin system. And this is another spin system, there are two spin systems here, which COSY will easily identify. So this what we started with, one of them is H2 and then it correlates to H1, and then also to H3. And of course in this region you can identify a methyl peak, and of course there is a cross peak between H8 to H7. And then of course other one, other also between 6 and 5 you will get the cross peaks. So easy. This is a crowded region, I did not explain this. This is very easy, I assume that I know how to make the assignment by using COSY, I can assign all the peaks. My main idea is to get the conformational information for this molecule using NOESY. This is the NOESY spectrum of the same molecule.



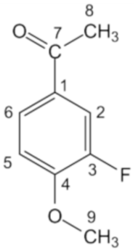


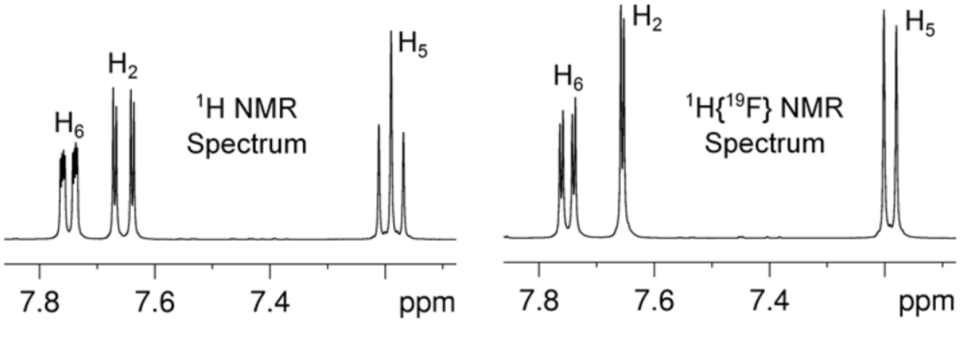
Of course you will see that the peaks are will not be exactly identical to COSY, because there will be additional peaks coming because of the NOESY. Again you can see there are correlations here from proton 3 to proton 1, and proton 3 to proton 5 here. What does it tell you? See proton 1 is correlated to proton 3, this is possible only when these two are on the same side of the double bond, of this double bond. Similarly CH2 correlated to H3 that also implies that these two are on the same side of the double bond. Wo these correlations are seen here. This is a correlation between H3 to H1 and then you also have a 3 to H5, both are being seen here. And this puts this CH3 and CH on the same side of the double bond. And further, you can also see the correlation between H2 to H1, this is H2 to H1 is there, and H2 to H5 is also there, that you can see here. H2 to H1 and also H2 to H5. What does this say? that means these are all on the other side of the double bond. So this clearly tells you, the NOESY cross peaks tells me this cross peak between these two puts them on the one side of the double bond, and cross peak between 2 and 3 here and of course 2 and 3 are trans to each other across the double bond. This confirms these alkene protons 2 and 3 are trans to each other, because these are one side, these two are one side, from the correlation information what we got from the NOESY spectrum. OK. The question is if the alkene were to be cis what would have happened? this instead of trans. We know correlation is between this and this, and between this and this, that is why we said these two are trans to each other. And these are one side of the double bond, that is fine. If they were not trans what would have happened? if they were to be cis then you would not get H2 to H5 correlation. This correlation you will not see, and you will not get H3 and H1 correlation. If it is on the other side distance becomes more you will not get the correlation. So, these type of correlations what we observe for this molecule puts these two on one side, and these two on other side of the double bond, and establishes cis geometry for the alkene group of this molecule. For the alkene protons it establishes cis geometry. This how we can understand, very easily we can interpret it.

We will extend further how we can get the information about the substitution at a particular site. If the site specific substitution is there in phenyl groups, how we can use NOESY. Tor that I have taken the example of 3'-Fluoro-4'-methoxyacetophenone. this is a molecular structure. We want to see, or our main idea is where is the OCH3 and where is this one? with respect to fluorine this one. Or in other words we need to get the structure of the molecule. Where is the position of fluorine this and this with respect to that. That information about the structure we should get. We can use various methods like COSY, NOESY, everything will adapt. Now, the first is you have to get a proton NMR spectrum, we need to analyze that.

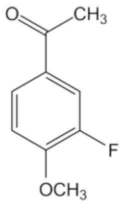


Of course, this analysis is not a rocket science, very easily you can understand. Looking at this one, of course, this proton 8 is COCH3 and of course, proton 9 is OCH3, directly attached to this one. This is a methoxy proton, this is just COCH3 group. And this is here, this is here, H8 and H9 and both of them are singlets. There is no long range coupling to this we are seeing. May be it is there, we are not seeing it. And the remaining thing is only these 3 protons, 1, 2 and 3. And they are all coupled to fluorine. Remember fluorine is a spin half nucleus, with 100 percent abundance. So, fluorine proton couplings are reflected in this spectrum. So, looking at the spectrum you can I try to understand or make the assignment which proton is which. Very easily you can do that. If you look at this proton, this one experiences only one ortho coupling it has to be a doublet, or this one experience only one coupling with fluorine, has to be a doublet. For example if you look at this one, this can experience a meta coupling, this can experience a para coupling, we can see varieties things. So, best thing is we will expand this and see the spectrum. It is a proton spectrum, of these 3 proton peaks are expanded. Look at it, very easily you can identify which is which. This is proton 5, the proton 5 is here. Why it is a triplet, of course, this has one ortho coupling with this and also meta coupling with this. If both of them are nearly equal it should be doublet of a doublet or if they are equal it will be a triplet. So, this could be H5, because it is equal. Now come to H2, H2 has one ortho coupling with fluorine and a meta coupling with this, para coupling may be there or may not be seen. So, it is a doublet of a doublet, I can clearly say that is H2. What about H6? The H6 proton will have a ortho coupling with this, and a meta coupling with this, and also a para coupling. In principle it should be doublet of doublet of a doublet, 8 line pattern. The large doublet is because of one of the ortho coupling, and then coupling with the fluorine, and then with this one. To simplify the problem what we can do is, we will do the fluorine decoupling. That is also possible heteronuclear decoupling we can do while observing proton. When you do the fluorine decoupling what will happen? we are going to break all the couplings of proton with fluorine. Only we will get HH couplings, FH couplings are completely removed. That is what we do, broadband fluorine decoupling of the proton spectrum and this is a fluorine decoupled spectrum.





If you look at it H5 is a doublet. Obviously this has to be this only, 3 bond ortho coupling between 5 and 6. Then H2, F coupling is broken, then it is only a meta coupling, so this is this. So I can clearly or conclusively say that is proton 2. Then what about the other one? other one is proton 6, proton 6 very easily you can identify. This is proton 6, it has one ortho coupling and meta coupling, doublet of doublet. A large doublet is because of ortho coupling and small doublet coupling is because of meta coupling, very easily you can do it by doing the fluorine decoupling. The same thing if you have little experience you can do without decoupling also. But this simplifies the spectrum. So now you have made the assignment of protons 2 ,5 and 6, for all the 3 protons in the proton spectrum, using both fluorine decoupling and non decoupled spectrum. And this is the spectrum and this comes because of J ortho I told you, J meta, this is J ortho plus J meta. Remember whe I analyze the proton spectrum of the molecules containing phenyl groups multiplicity patterns, how it comes I explained to you. Based on ortho coupling, meta coupling and para coupling what type of pattern we get, using that knowledge here we can completely make the assignment. All right, from the coupling pattern and using this one also, we know this compound look at it, this one ortho, one meta, and one ortho and meta coupling, is there. Looking at how this type of splitting arises, you can come to a conclusion this must be 1,2, 4 tri-substituted, because here look at it, here if it is 1,2, 4-tri-substituted. See what will happen? this is 1, 2 and 4 tri-substituted. If that is the situation only then this pattern will come, because of ortho, meta and para couplings, what we saw here. This pattern is possible only if the substitution is 1,2, 4 tri-substituted benzene. Which substituent is in which position is a different question. But the three places at which in the phenyl group substitution comes is at 1, 2 and 4. Ok. Then find out the possibilities. We know the structure of this molecule is given. There are various possibilities 1,2, 4, this could be one possibility, 1, 2 and 4, fluorine instead of here could be here, and 1, 2 and 4, fluorine is here. And these two are ortho to each other. Think of all the possibilities. There are six such possibilities we can think of, for 1,2, 4 substitution where one is fluorine other two substituents are OCH3 and COCH3. This is the situation, so there are six possibilities we think of.



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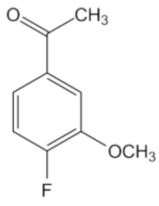

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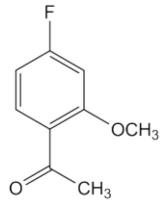

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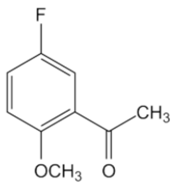

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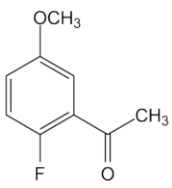

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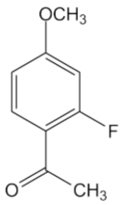

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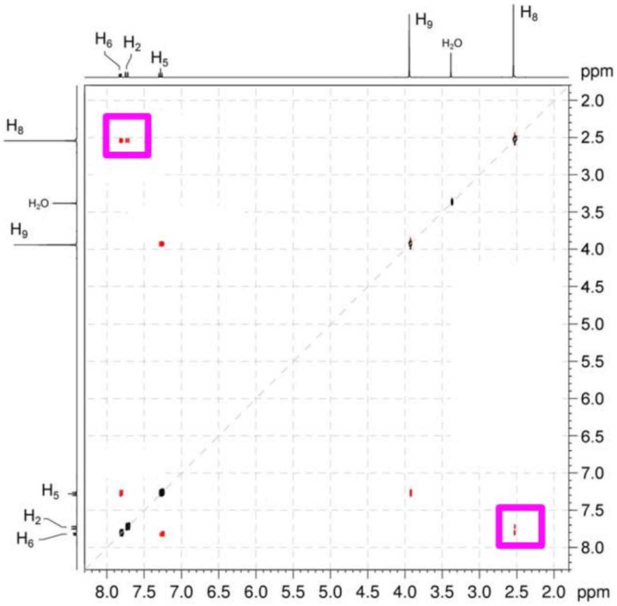
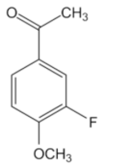
Now let us look at the NOESY spectrum. Assuming that we know all the assignments, and that have already been made, let us look at the NOESY spectrum.



In the NOESY CH3 protons show correlation to two protons H2 and H6, we already made the assignment. This is H2 and H6, here this one H2 and H6, both are close by and NOESY is giving me cross peak, especially the CH3 proton. This is the CH3 proton, not OCH3. OCH3 comes down field I told you, So this CH3 proton is giving cross peak to two protons, that means what is the conclusion you are going to draw? This tells me that this group must be between two protons of the phenyl group. It cannot be one like this, it is not possible. It cannot be here because other side is this one, it must be between two protons of the phenyl group, that is because of the correlations 2 and 6 are seen for CH3 group. This places the acyl group between two protons of the aromatic protons. So what are the possibilities we can think of. There are six possibilities, then if this has to be between two protons, then this is not possible, this is not possible, this is not possible, this is not possible. So all four possibilities are ruled out.



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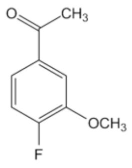

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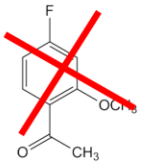

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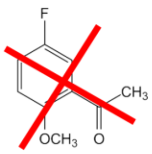

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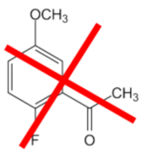

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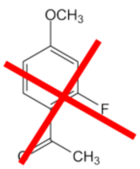

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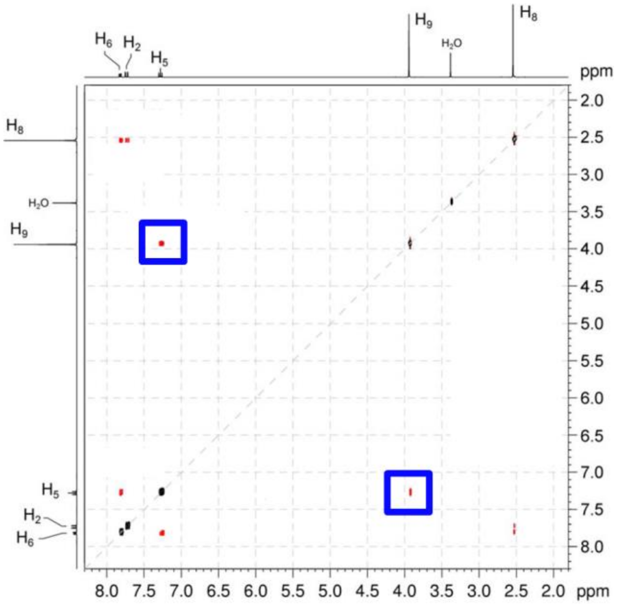
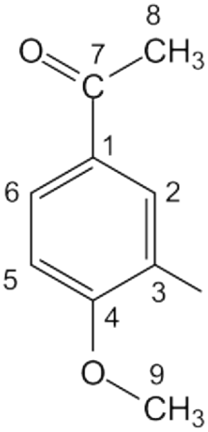
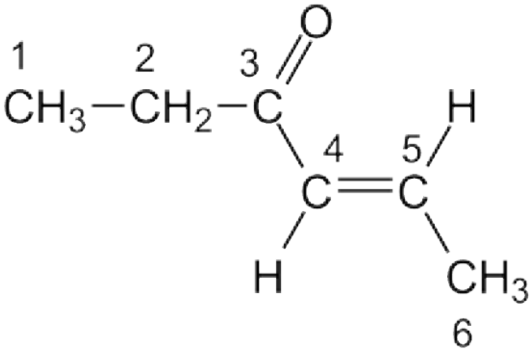
Then we are left with only two possibilities, because CH3 has given cross peak to two protons either this should be this or this. Only here this position is changed that is all. That is the only possibility where OCH3 can be between two protons. Now there are two possibilities. We will go further down. Look at the NOESY spectrum, again.



We look at OCH3 protons, OCH3 this proton gives cross peak to proton 5 which is at 7.2. This one see, it is giving a cross peak to OCH3, this is OCH3. See from the diagonal come here, go here, and then compute this square. So this OCH3, it is giving a cross peak to only one phenyl proton. That means what is the possibility we can think of. Then this will be the only possibility, fluorine is on the right side. It is not giving correlation to that, so that means if you consider this possibility, already we have eliminated this, now this is also eliminated, because if this is the fluorine OCH3 cannot give correlation to this. This is the only possibility it can give correlation to this so fluorine, cannot be here. The fluorine has to be on other side, here. It cannot be here, okay, That is what is the conclusion. So this also is ruled out. Then what? The OCH3 protons must be ortho to H5 proton. That is what the conclusion, otherwise OCH3 cannot give correlation to this. So OCH3 proton is ortho to H5 proton. Using this NOESY information we can draw the conclusion now. This is the structure of molecule, because we understood this is between two protons, and this is giving cross peak to this one alone. That confirms this is the structure. All other possibilities are ruled out. So beautifully using the NOESY you can get the conformation. I hope you get the point.

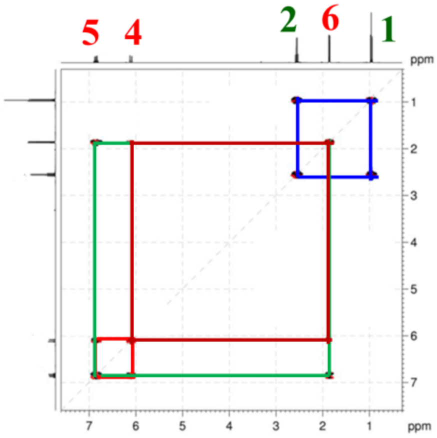


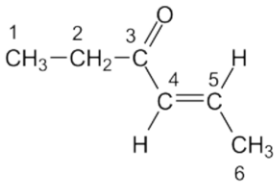
We will go further. Let us look at the another molecule.



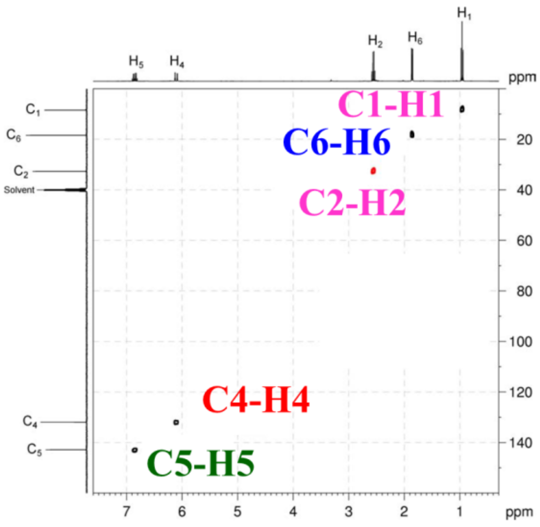
This is a molecule we will use all the possible techniques in 2D like, COSY, HSQC, HMBC, NOESY etc and get the structure of the molecule. I am showing you all these things, but you know if you are little bit of experienced person, if you already worked in the NMR for couple of weeks or months, then all you do not require. You know 1D NMR, COSY is not required, HSQC is not required. Looking at the simple molecule and proton NMR spectrum it will be fairly easy enough to for you to analyze and get the information. But to make you comfortable, to comfort all of you, I am going through all these 2D spectra, so that you know what are the steps you have to follow to analyze this spectrum.

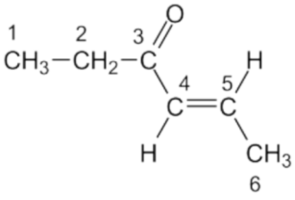
Of course this is a proton-proton COSY, very easily you can anlayse that. This is proton 1, this is CH3-CH2, an isolated group here. This is triplet and this is a quartet. This is correlated to this. This is the only isolated group, no other correlation. So COSY identified this, and then and next is this one. We start with this CH3.



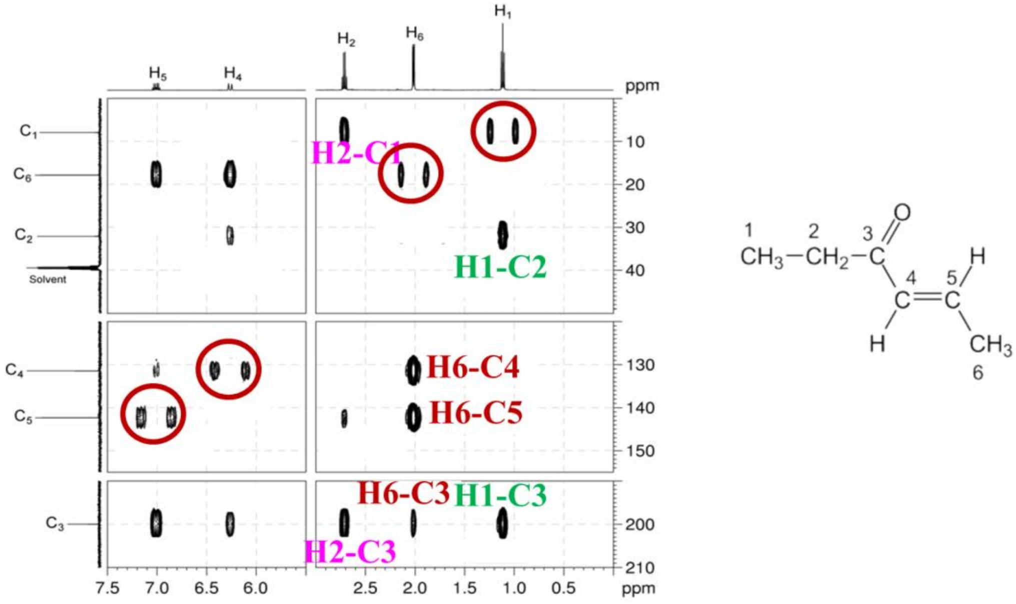


This is CH_3. Come down and it correlates to two protons which are here. And again this is correlated to one of them, this will correlate within itself, the other one. So 4 and 5 are correlated, and both of them are correlated to 1. Very easily you can identify which is which. And of course further to find out the number of carbons and everything whether it is CH2 proton or CH3 proton, because we need to identify whether it is CH2 or not by looking at the multiplicity pattern, triplet and quartet you know you one is CH2 or there is CH3. Just to make you understand where we can utilize multiplicity edited HSQC spectrum.

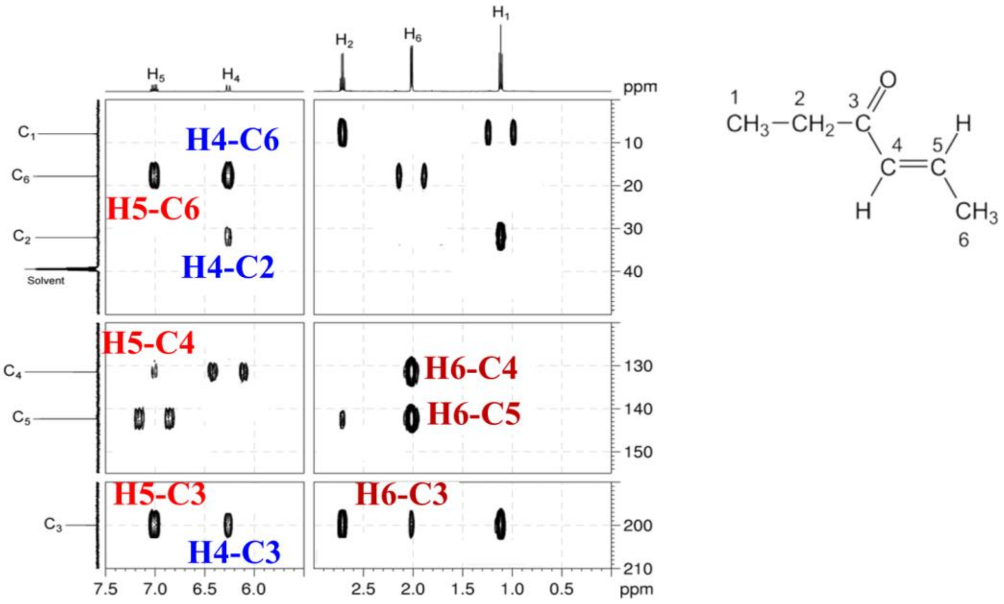




If you do that, you see the opposite sign here, that tells me proton number 2 must be CH2. Very easily you know that. Fine, that is what it is. And you know the correlations. From this which are the carbon chemical shift which are the correlations everything you can identify. There are only five protons here five, different correlations we are seeing. Of course this carbon you are not going to see. To confirm there is one CH2 by this multiplicity edited HSQC. Of course we can also do HMBC to get the carbon-carbon correlation. Of course that is not needed, if you want to get the structure. I am looking at only whether this is trans to each other or cis to each other. For that we do not require HMBC. But for the sake of showing, I am showing you.

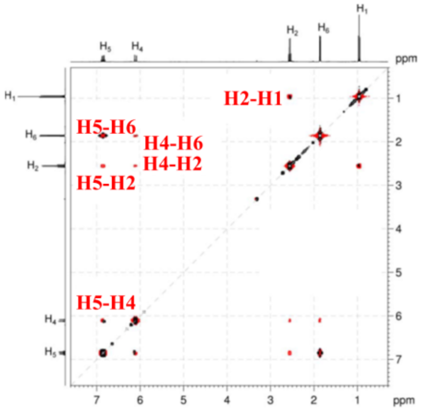


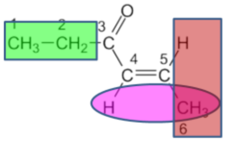
Sometimes it so happens you will get large cross peaks, which are widely separated like this. They are all one bond HSQC correlations, they are not efficiently filtered out. In HMBC I told you one bond HSQC correlation peaks are filtered out, but if they do not filter out efficiently you see all of them. Here there are four such correlations, all right.



And then you can see HMBC, H1 is correlating to C2, this is correlating to C2, and H1 is also correlating to C3. This puts them on one side of the C=O, okay. See H2 is also correlating to C1, H1 is correlating to C2, H1 is correlating to C3, H2 is correlating to C1 and H2 is also correlating to C3. So varieties of correlations you can see. This puts the CH3-CH2 on one side of C=O. That is what we can say. We can say CH3-CH2 is attached to C=O from these correlations, HMBC correlations. I hope it is clear for you. So remember there are correlations what you have to see. Here this is correlating to this carbon, this is also correlating to this, and this is correlating to this carbon, like this. This gives me the idea that CH3-CH2 is attached to C=O. All right, we will go further. Now we can also see H4 correlating to C6, H4 correlating to C2, H4 correlating to C3, all these correlations we can see. Similarly H5 correlation, 3 carbons it correlate. Similarly H6 correlate to 3 different carbons. All these tells me that this group is on other side of the C=O. If we carefully go through it one by one, slowly we can see that one. But anyway that tells me that now there is a C=O. These are on one side and this is one the other side. So some sort of an information about the molecular structure is known.

400 MHz ^{1}H–^{1}H NOESY spectrum of *trans*-4-hexen-3-one

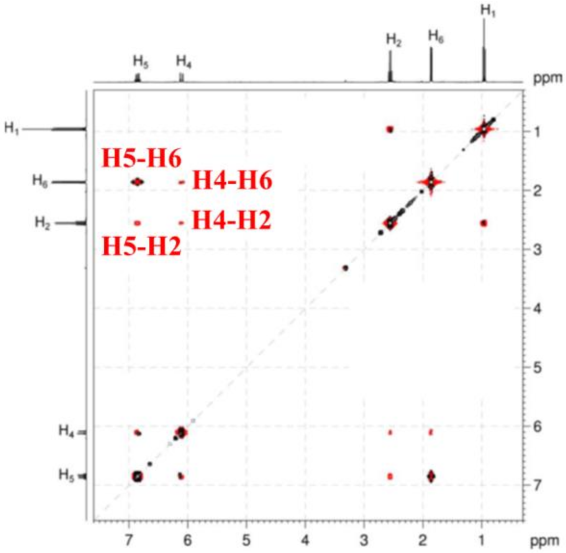


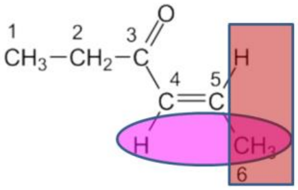


Six correlations

H2 → H1, H4 → H2,
H5 → H2, H5 → H4,
H4 → H6, H5 → H6

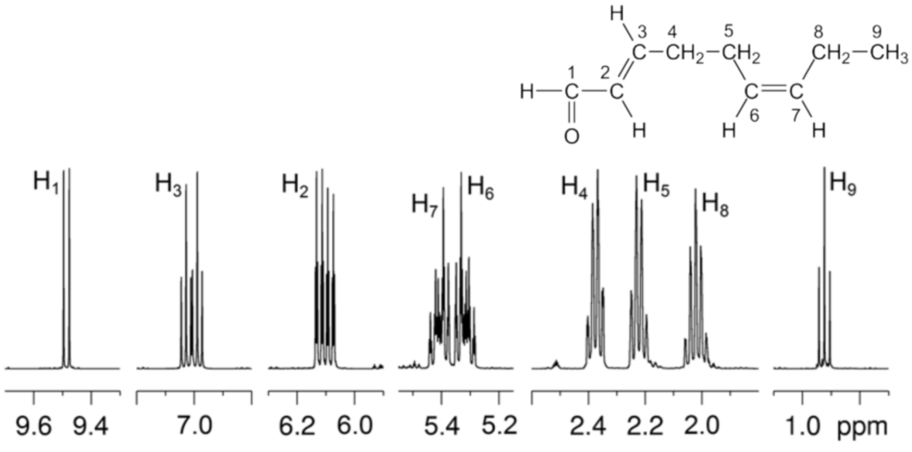
We will use the NOESY now further, to get the conformation. Basically what you need to know is whether these are trans or cis to each other. And if you see the NOESY, there are several correlations here. one CH3 to CH2, this one is there, this correlation. H2-H1 correlation is there. And H4-H6 correlation is there, this is fantastic. This H4-H6 correlation here easily tells me that H4 and H6 are on one side of the double bond. Whereas, H2 is correlating to H1, they are on other side and then further you are going to get H4-H6 correlation, H5-H6 correlation is seen, H5 H2 correlation is seen. See here, H5-H6 and H5-H2 correlations are seen. What does it tell you? All these six correlations if you see, if you see H2 correlated H1, H4 to H2, it tells me this is on the other side of the double bond. Similarly these correlations tell me, for example, H4 and H6 correlation tells me these four are on one side of the double bond.



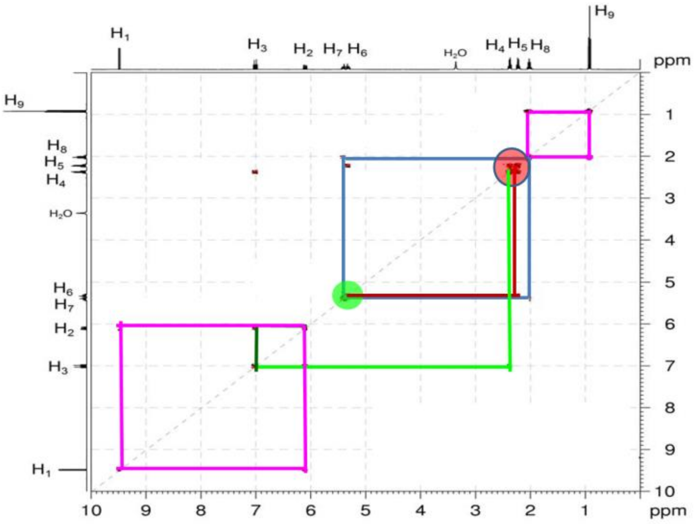


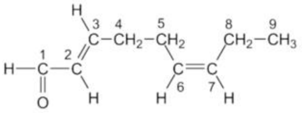
So the all these correlations tells me now this, then this, and this correlation, H4-H6 indicate it is a trans geometry. H4H6 correlation and this correlation and this correlation tells me they are in the trans geometry. If they were to be cis you would not have got H4-H6 correlation. So that is the thing. So this what it is. This indicates the trans geometry for this alkene functional group. So now you know H4-H6 and H5 correlation and H5-H2, this correlation would be absent if this group were to be cis, because this H would come here then C8 would be here, then this H5 and H2 correlation would not be seen. Similarly, H4H6 correlation would not be seen, because this will be trans to this one. This type of observation tells me that these two protons, alkene protons are trans to each other, and not cis to each other. So from both observation of the peaks and non-observation, if in case if it were to be cis you would not have seen that, we can come to a conclusion what is the structure or geometry of this molecule.

We can go further for this molecule. Another one, this is a very simple spectrum.

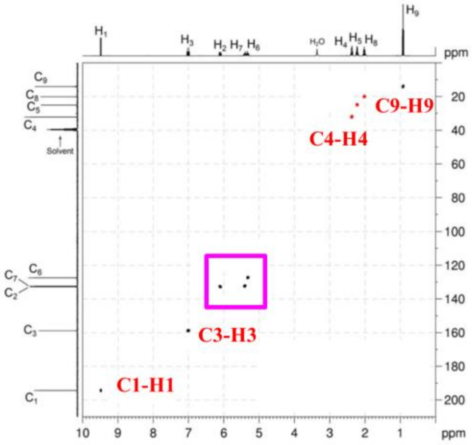


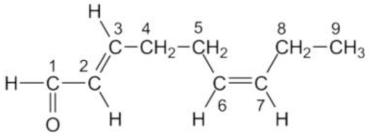
Look at it, we have proton 9. This is easily analyzable. We analyzed this in the 1D, 2D, COSY also, I remember. So we can start looking at the COSY spectrum.



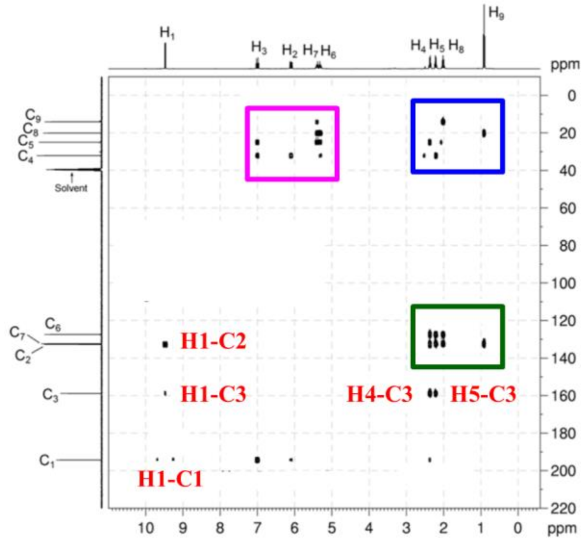


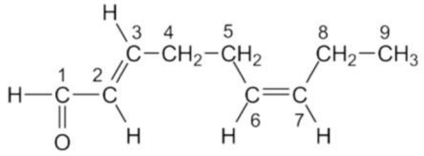
The COSY specturm identifies this one, H3 to H2 correlation. And from H2 we can go to this. They are numbered 8 and 9, then so 9 to 8, 8 to 7 it comes, and then here 7 to 6 is there, from 6 you can go further, and you will identify 5. From 5 you can go to 4, from 4 to 3 like that, entire specrum, all these protons could be assigned. Just by systematically going step by step, I did this step by step. You can slowly see, it I will show you again. See 9 is I identified, the peak 9 which I am confident. From 9, I will go, it correlates to 8, from 8 it will go to 7, 7 to 6 is there, 6 to 5 it goes, from 5 to 4 is correlated here itself, and 4 to 3 is here, and 3 to 2 here, and 2 to 1 here. Everything you can assign without any difficulty. Alright. Of course, multiplicity edited HSQC confirms how many CH2s are there.





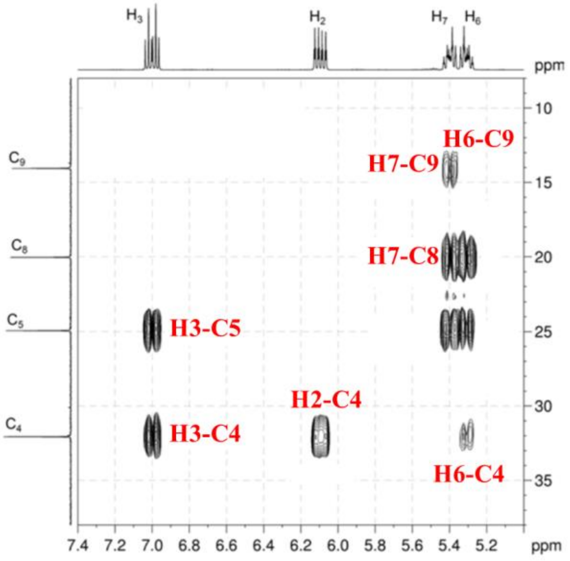
There are here 3 red peaks, you can see negative peaks, that shows there are 3 CH2s in this molecule. And of course, you can start looking at the HSQCC and make the assignment of all the carbon proton, correlations.

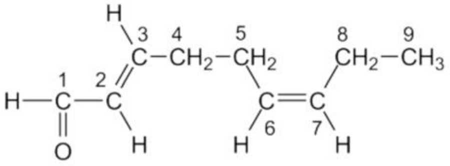


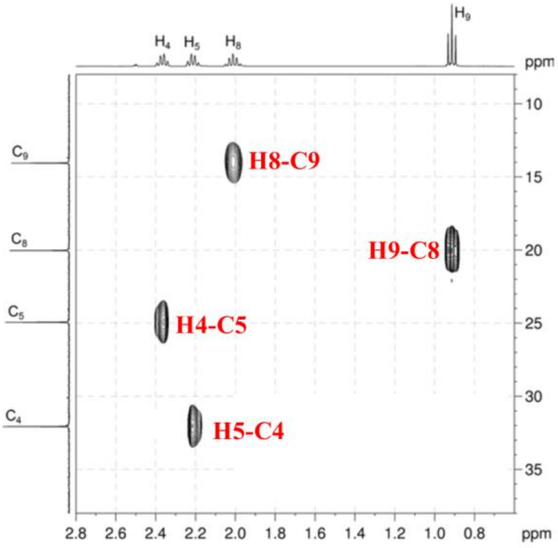


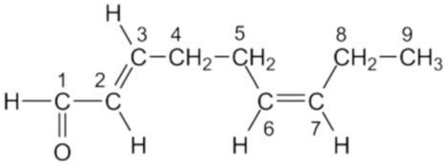
H1-C1 is HSQC peak ($(^1J_{CH})$)

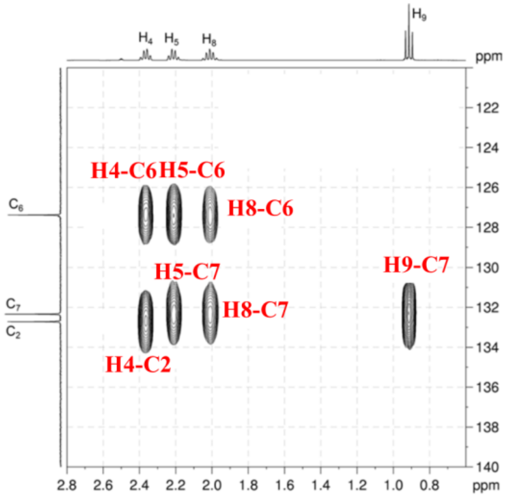
Here H1-C1 here, and then H2-C2, H1-C3, H1 is correlating to C1 C2 and C3 and H4 is correlating to C3 and H5 is correlating to C3. So, all this information if a couple you will find out what is what. Completely we can make the assignment of every peak here. I will not go step by step, very easily you can do. Of course, I have already told you how you can analyze the HMBC spectrum. Just I wanted to show that we can using this HMBC and all these expanded regions, with all the correlations here you can identify and get the structure of the molecule, the carbon skeleton of the molecule.

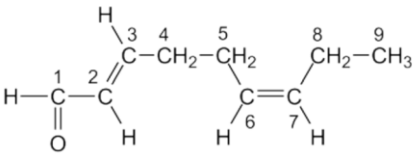






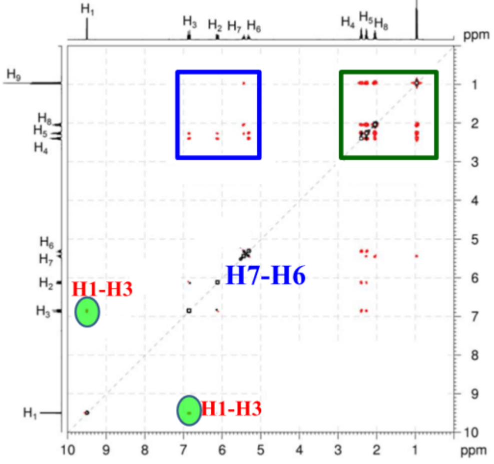


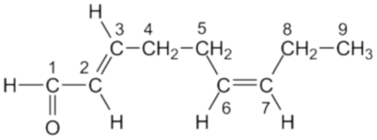


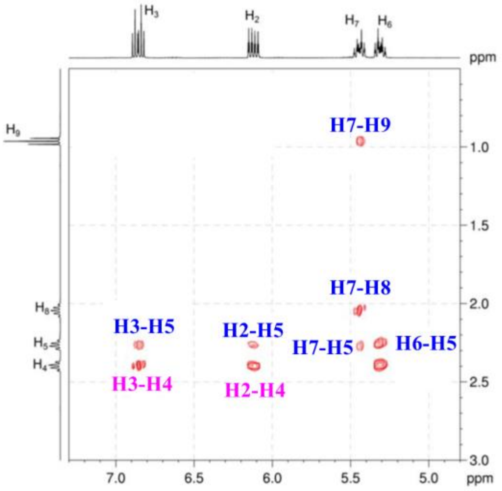


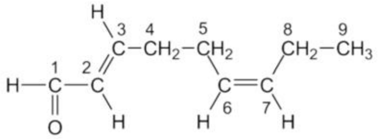
More than that now you got the proton assignment, carbon skeleton, carbon chemical shifts everything. But finally, what is left is the confiomation of the molecule.

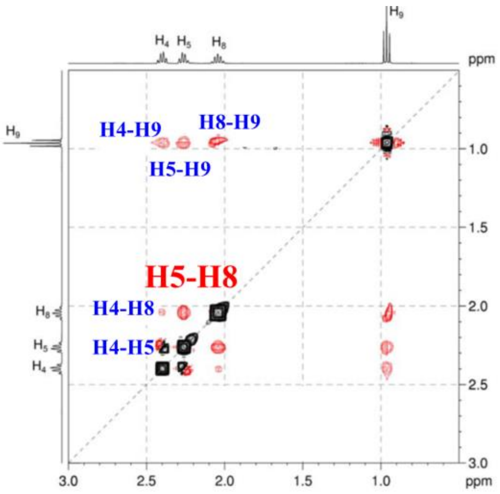
NOESY spectrum of trans-2,cis-6-Nonadienal

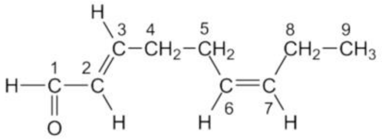








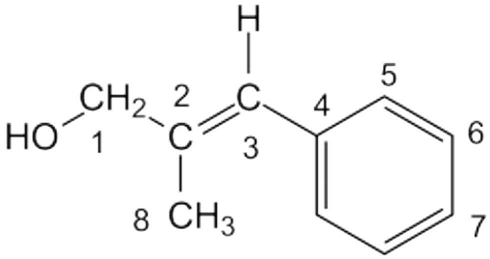




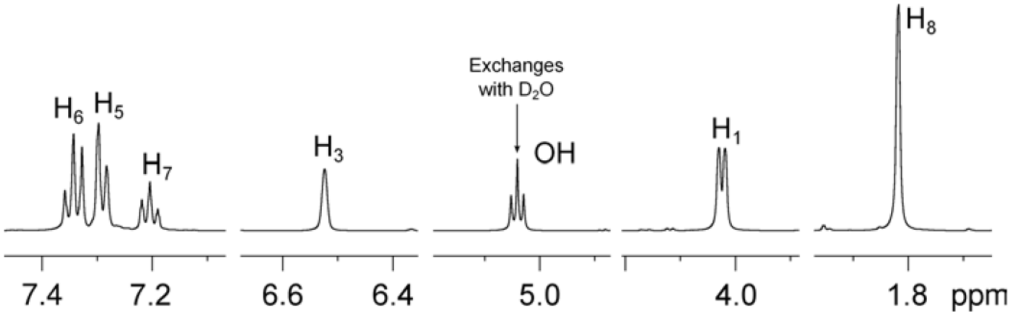
Here we use NOESY. You can see from the NOESY, the H1 and H3 correlations are there here, see H1 and H3 correlations are there. This H1 and H3 correlation says that they are on the same side of the double bond. If this was to be here you would not see correlation for H1 and H3. If it were to be cis, because these are on the same side of the double bond you are seeing the correlation. So, H1-H3 correlations are seen. Similarly H7-H6 correlations are seen. This also tells me they must be on the same side of the double bond. When you say these two on the same side of the double bond this must be a cis geometry. You have got the information already. And you can expand this further you can see H1 is correlated to H3, and H3 to H5. This is correlating to this one, and H2 is correlating to H4 here. See this should be on this side if it was to be there, if on other side, it would not give correlation to H4. So, all these things indicates this is a trans geometry. Whereas this is cis geometry, you understand the point.

Now, correlations of NOESY tells me this double bond if you consider, the protons 2 and 3 are trans to each other. Whereas looking at the correlation of 6 and 7, I can say proton

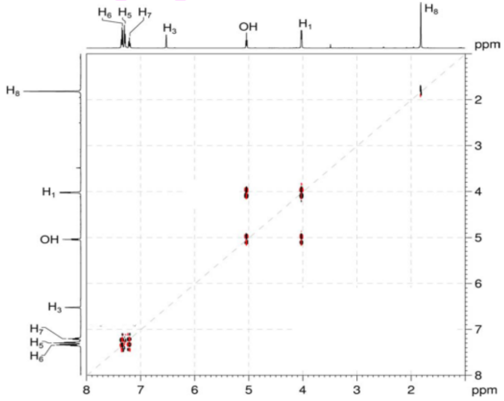
6 and 7 are cis to each other in this molecule. The H5 H8 correlation places two CH2 groups on the same side of the double bond here. In addition to 6, 7 we also see 5 8 correlations here. This 5-8 correlation you can see here, this is. So, this tells me when I see that 5-8 correlation these two CH2 groups on one side. The 6-7 correlation tells these two on one side, and this correlation tells me these are on the one side of the double bond. And these two tells me they are cis to each other. So, varieties of correlation information you could get. So many correlation peaks, all these things put together in a nutshell we can say this molecule has one double bond with a trans geometry, and another double bond with a cis geometry. This is the structure of the molecule. So, we can get the structure of the molecule very easily like that. Of course, we can continue further. One more molecule we will see.

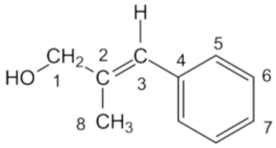


And I will quickly show you, this is the 1D spectrum. very easily you can analyze this one. There is no difficulty.

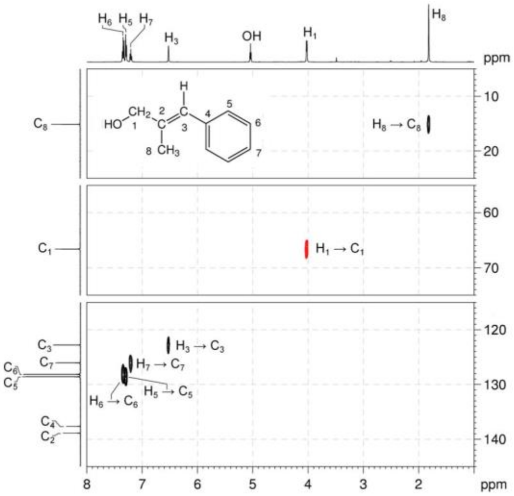


1H–1H COSY spectrum of *trans*-2-methyl-3-phenyl-2-propen-1-ol (DMSO-*d*6, 500 MHz)



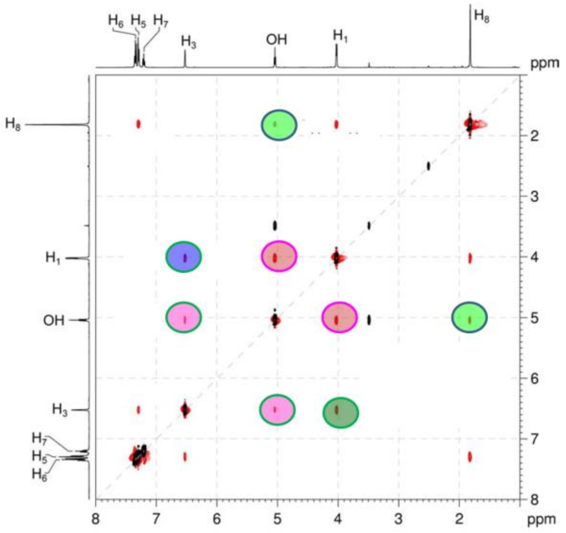


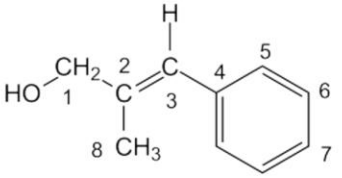
Take the peak, COSY peak here, these are all phenyl protons. From the COSY you can identify. And this is the phenyl group, these two are correlated to each other. Rhen there is a correlation among only these groups, here you can see that. All right, you can use multiplicity edited HSQC to identify whether there is a CH2.



There is only one of them is red in color, negative sign, which tells me this H1-C1 is correlated, and H1 this, might be CH2. With that information now we go to NOESY.

1H–1H NOESY spectrum





OH correlates to H1 and H8

H3 correlates to H1 and OH

Indicates CH2 and OH are on the same side of double bond

This is where clear information you are going to get. OH correlates to H1 here, this is a OH proton. This correlates to H1, OH is here, it is correlated to H1 here, you see there is a correlated peak. These two are correlated. And then, also OH is correlated to H8. This one. This tells me these two are on the same side, especially close to each other. H3 correlates to H1. Which is H3? H3 is here. See H3 correlates to H1, and OH. both. It also correlates to OH. When H3 is correlated to OH and H1, that means this CH2 and this proton are on one side of the double bond. This clearly tells me, this correlation tells me this CH3 is on the other side of the double bond. This correlation tell me CH2 and H are other side of the double bond. So, like this you get the correlation information. This indicates CH2 and OH are on one side, and these two protons. this correlation tells me this is on other side, this CH2. Also further you can go H8, this one, is correlated to H5, because these two are symmetric, I have not written here, but this is also same. This CH3 is correlated to aromatic proton, H5, That clearly tells me these two are trans to each other, because there is a correlation between this and this, and there is no correlation between this and this. There is a correlation between CH3 and this proton, aromatic proton. All these tells me, then CH3 and alkenes are on the same side of the double bond. So, this clearly gives me the idea about the geometry of this molecule. And this is the geometry. And there is no correlation between H3 and H8, this and this there is no correlation, because they are trans to each other. Very easily you got correlation between this and this, you got correlation between this and this, you got the correlation between this and this, that is all. Very easily using this information you can fix the geometry of this molecule. That tells me CH3 and H are trans to each other. And of course, this is how we can analyze structure of the molecules. And I think we took good number of examples. What I am going to do is stop here. In this class we have discussed, and taken several examples of simple molecules, to show how we can utilize, by the combined use of all the 2D technique like COSY, HSQC, HMBC, NOESY, we can get the structure. Sometimes all are not needed, in some cases you require them. Just if you are a beginner you should go through all the things, all the spectra so that you know how to go systematically. Or if you are already a person working with NMR and with little bit of experience, and for couple of weeks or months if you have worked, you do not need everything. Just by 1D spectrum or COSY you will get some information, straight away you can go to NOESY. Based on the correlation information you could get structure of the molecule. So, we could get several examples of the molecules, which have got a double bond, where you could get the cis-trans geometry information, and in the phenyl group you could find out the substitution position, and rule out all other possibilities by just by using NOESY. So, these are some of the examples. I will stop here we will continue with few more examples and other topics in the next class. Thank you.