NMR Spec

Transcript

Instructor: Clara

00:00:00:00 - 00:00:05:12
Instructor: Hi, everyone. On today's video, we're going to talk about how you would target NMR problems.

00:00:05:12 - 00:00:16:68
Instructor: We know that NMR is all about giving hints and how your atoms are displayed in your molecule. We know we have different types of NMR, and then today, we're going to be focusing on your hydrogen NMR.

00:00:16:68 - 00:00:29:04
Instructor: We know that those peaks come from every interaction that the hydrogen is going to have around your molecule, and normally those peaks come from your hybridization, polarity, and different types of groups that you might have around. This gives us our chemical shift.

00:00:29:04 - 00:00:37:08
Instructor: We're going to dive a little bit deeper onto what our chemical shift looks like and what are patterns that we can see. To get a deeper look at chemical shift.

00:00:37:08 - 00:00:49:53
Instructor: We can look at this blank spectrum and see what patterns we're going to look for. So around one and two PPM, we're going to see our CH three showing up and our CH two.

00:00:49:53 - 00:01:04:09
Instructor: These are very easy to identify. Those peaks are normally very at the beginning compared to the other ones, and then from our four to five, we're normally going to see some alkenes in our electron withdrawing group.

00:01:04:17 - 00:01:15:33
Instructor: Okay. For the alkenes in electron withdrawing group, remember that they show up a little bit more downfield and we're going to talk a little bit more about that.

00:01:15:33 - 00:01:28:05
Instructor: Then from our seven to eight, it's our classic aromatics. Then 9-10, we have our aldehydes and 11 to 12 are carboxylic acid.

00:01:32:39 - 00:01:49:35
Instructor: Remember, you don't have to memorize these, but these are going to become patterns that you're going to be used to, and as soon as you see them, you're going to be able to identify those peaks. Now we're going to go through a to do list on how to target NMR problems, and this should be a pattern with all of the examples that you guys are going to do.

00:01:49:35 - 00:02:01:37
Instructor: The first item in our list is to count the peaks and look at your chemical shift. Remember that the number of peaks that you have in your spectrum is equal to the number of different environments aka, different Hs that you're going to have.

00:02:01:37 - 00:02:06:69
Instructor: We talk them as being chemically equivalent. Not all Hs in your molecule are chemically equivalent.

00:02:06:69 - 00:02:16:97
Instructor: That's where your different peaks come from. Just a couple examples as a reminder, this one, we say that all three of them are chemically equivalent, which yields one peak.

00:02:16:97 - 00:02:37:63
Instructor: For the second example, we have two different environments going on for those Hs that we have, meaning we're going to have two different peaks in our spectrum. For our last example, we're also going to have two peaks and remember that OH for your alcohol is also a different peak and normally comes in a broad single peak.

00:02:39:87 - 00:02:54:60
Instructor: Remember for number one in our list, count your peaks and remember the different environments that you're going to have and they match your number of peaks. Our second item in our to do list is to look for any special atoms or any electron withdrawing groups.

00:02:54:60 - 00:03:05:24
Instructor: Remember that your magnet in your NMR always tries to push downfield. Any hydrogen atoms that may be close to your electron withdrawing groups may show up in a peak that's a lot more downfield than what you're used to.

00:03:05:24 - 00:03:27:08
Instructor: For example, on this one, your hydrogen alone is going to show up at the beginning, like we talked about, but on this example where you have an oxygen close to it, your peak is going to show up a lot more downfield. Remember that those electron

withdrawing groups will withdraw electron density away from the hydrogen which will be more susceptible to the magnet, meaning that that peak from the hydrogen will show up a lot more downfield.

00:03:27:08 - 00:03:43:53
Instructor: The movement of the electron density goes from your hydrogen towards your oxygen because withdrawing that. So now we have a lot more electron density around the oxygen, leaving the hydrogen susceptible to the magnet.

00:03:43:53 - 00:03:56:01
Instructor: So remember to look for those electro withdrawing groups that may skew your spectra a little bit and move those peaks downfield other than the ones that you're used to seeing. For a third item in our to do list is for you to check your integration.

00:03:56:01 - 00:04:16:98
Instructor: Remember that the integration number you're going to see means the amount of hydrogens that are chemically equivalent in that peak, meaning that if you have an integration of two, this is most likely a CH two because those two hydrogens are equivalent in the molecule and they yield one peak. If you have an integration of three, this is most likely a CH three.

00:04:16:98 - 00:04:39:59
Instructor: For your integration of six, this can be that you have two times a CH three, which means that those CH three at the end of your molecule are chemically equivalent and are going to yield one peak, or you may have three times a CH two. Remember that this is not as common, but still may happen and you have to take into account the pieces that you're putting it together.

00:04:39:59 - 00:04:48:41
Instructor: So for the third thing you're doing your to do list is check your integration, and that will help you piece everything together. The last item in our to do list is to check your splitting.

00:04:48:41 - 00:04:57:53
Instructor: Remember the N plus one rule and where that's going to come into play. This hydrogen in the middle with the CH2, they're going to integrate for two as one peak.

00:04:57:53 - 00:05:06:05
Instructor: However, they're going to split as a quartet due to the three hydrogens beside it. Okay. And then for

00:05:06:05 - 00:05:26:19
Instructor: second peak because we have two different types of hydrogens, for this one, it's going to just split as a triplet because it feels itself plus the two hydrogens beside it. Now having your splitting and your integration, it will help you piece your molecule together based on all those hints that you just gathered.

00:05:26:59 - 00:05:35:27
Instructor: For this example, we're giving a molecular formula and your spectra. Remember that we have our to do list up here and then we're going to follow it through.

00:05:35:75 - 00:05:42:25
Instructor: Our number one in our to do list is to count the peaks. You have 3 different peaks, aka 3 different environments.

00:05:42:25 - 00:05:46:31
Instructor: One thing I want to point out is that broad singlet around two to 2.5.

00:05:46:31 - 00:05:54:77
Instructor: Normally, when we see broad singlets it means that we have an alcohol. Also, remember that the 3.6 peak is very much downfield,

00:05:54:77 - 00:06:13:06
Instructor: which indicates it's most likely close to that OH that you just found out. For our second item in our to do list, we know that we have an oxygen, that will bring it more downfield, which makes sense with the first point that we did for the 3.6 PPM peak.

00:06:15:26 - 00:06:24:82
Instructor: For a third item, we know that we have to look at integration. For the first peak it integrates for three, which is most likely a CH three.

00:06:25:82 - 00:06:39:20
Instructor: For a second peak which integrates for one, it makes sense to be ROH, which only has one hydrogen. Lastly, for 3.6, we know it integrates for two,

00:06:39:20 - 00:06:44:28
Instructor: which is most likely a CH two. Okay.

00:06:44:28 - 00:06:55:46
Instructor: Now that we have all of our pieces, we need to connect them through our fourth item, the splitting. Remember that the splitting is going to tell us the order of stuff and where they're going to connect.

00:06:55:46 - 00:07:00:10
Instructor: For the first one at 1.2, it splits as a triplet.

00:07:01:90 - 00:07:09:86
Instructor: Then for two to 2.5, it's a broad singlet, meaning it doesn't have any neighboring hydrogens around it.

00:07:11:76 - 00:07:19:20
Instructor: And lastly, for 3.6, it's split into a quartet, meaning there's three hydrogens around it.

00:07:19:20 - 00:07:36:96
Instructor: Now that we have our pieces and all the information are connected and makes sense, we can put those things together and make your molecule. Knowing that our CH three normally goes at the end and our OH is closer to our CH two, which was more downfield, you can put those two together.

00:07:37:96 - 00:07:52:82
Instructor: So there you have your molecule from your three pieces completing the splitting and how they are connected. It makes sense for this one to be more downfield as it's closer to the oxygen and this one more upfield as it shows up at 1.2 PPM.

00:07:52:82 - 00:08:08:60
Instructor: Now we can also double check our splitting. We know that the CH three is splitting as a triplet because of the neighboring two hydrogens and that CH two is spitting as a quartet because of the three hydrogens and that your CH two is splitting as a quartet because of the three neighboring hydrogens.

00:08:08:60 - 00:08:19:46
Instructor: Normally, our OH shows up at a singlet brought peak, even though they're neighboring hydrogens. For this example, we're going to take a look at this spectra and this molecular formula.

00:08:19:46 - 00:08:27:36
Instructor: Remembering following our to do list, we can take a look at the peaks. From our chemical shift, we can tell that the 7.2 PPM is most likely

00:08:27:36 - 00:08:34:80
Instructor: an aromatic and the beginning at 2.4 is also most likely either a CH two or CH three.

00:08:40:99 - 00:08:57:31
Instructor: Also, remember that we have two different peaks, meaning two different types of hydrogens. For number two, we can notice that there's no electron withdrawing group or any special atoms.

00:08:58:15 - 00:09:06:43
Instructor: Therefore, we can jump to number three, which is our integration. We can see that the 2.4 PPM peak integrates for three,

00:09:06:43 - 00:09:19:91
Instructor: most likely being a CH three, and that our 7.2 multiple, which is an aromatic integrates for five, meaning all five hydrogens in your atomatic in that case are chemically equivalent.

00:09:25:87 - 00:09:35:09

Instructor: For a last item in our to do list, the 2.4 PPM peak is showing up as a singlet, meaning there's no neighboring hydrogens.

00:09:35:09 - 00:09:39:91
Instructor: At our 7.2 PPM, which is aromatic normally comes up as a multiplet.

00:09:39:91 - 00:09:59:21
Instructor: There's a lot of electron density going on, which doesn't show up as very clean peak but still shows and tells us that it is an aromatic molecule. With this in mind, now we can build our molecule and tie those pieces together.

00:09:59:21 - 00:10:17:95
Instructor: We can start with our ring and knowing that our molecule has CH three and the remain is for the aromatic, we're going to do a hexagon. Knowing that all five hydrogens in that hexagon are equivalent, your stage three can go in any position.

00:10:18:28 - 00:10:40:64
Instructor: Having this as your final molecule, it ties all together with the CH three that we have as a singlet and our aromatic as a multiple. Notice that from this molecule and all the Hs being equivalent, we do have a mirror plane, which this is what allows all the Hs to be indistinguishable and chemically equivalent.

00:10:41:16 - 00:10:57:44
Instructor: In this example, we're giving a spectra with only one peak in this molecular formula. Looking at our to do list and looking at the peak, we know that by having only one peak, all the hydrogens, all the six hydrogens in the molecule are all chemically equivalent.

00:11:00:56 - 00:11:09:74
Instructor: Looking at number two, we do have an electron withdrawing group, the oxygen in our molecular formula. This means that that peak showing up at 2.1

00:11:09:74 - 00:11:30:38
Instructor: is most likely a lot more downfield than it would show up, meaning it could still be a stage three or a CH two. Then now looking at our only peak, the integration is six, meaning that single peak is equivalent to six hydrogens.

00:11:30:38 - 00:11:37:88
Instructor: Remember, that six hydrogens could be two times a stage three or three times a stage two. A.

00:11:41:23 - 00:11:52:67
Instructor: Now looking at number four in our list is the splitting. That peak is a singlet, meaning all six hydrogens are equivalent and do not have any neighboring hydrogens.

00:11:58:51 - 00:12:10:87

Instructor: Now that we have all of our pieces together, we can start building our molecule. Also remember that in any spectrum that you have very low numbers of peaks, it means that your molecule is very symmetrical.

00:12:11:15 - 00:12:32:75
Instructor: With this in mind, we can start placing all of our carbons in a chain and start filling in the gaps and seeing whether we have two CH threes or three H twos. Look at our formula and knowing that we still have an oxygen to place to maintain symmetry, we should place the oxygen in the middle and then we'll fill out in the blanks.

00:12:33:11 - 00:12:58:23
Instructor: With this in mind, we only have two carbons left, meaning we do have two CH threes instead of three CH twos. Then having your molecule complete, you can see your mirror plane right in the middle, making the molecule very symmetrical, yielding only one peak as those six hydrogens are all chemically equivalent.

00:12:58:23 - 00:13:06:75
Instructor: For this example, we're giving this spectra and this molecular formula. Remember our number one in our to do list is to count the peaks.

00:13:06:75 - 00:13:14:19
Instructor: We have three different peaks, meaning three different environments. Taking a look at that peak, that 1.2 is most likely

00:13:14:19 - 00:13:20:51
Instructor: a CH three as it's right in the beginning, and for 4.1 is a little bit more downfield.

00:13:20:51 - 00:13:27:13
Instructor: Maybe it's close to an electro withdrawing group. And taking a deeper look at that 11.0,

00:13:27:13 - 00:13:48:56
Instructor: it's most likely a carboxylic acid remembering our chemical shift. Now that we know we have a carboxylic acid, we do know that we have two oxygens acting as an electron withdrawing group, making those peaks more downfield to anything that's close to it.

00:13:50:96 - 00:13:58:06
Instructor: Now looking for number three, we look for integration. For our first peak at 1.2, integrates for three,

00:13:58:06 - 00:14:05:32
Instructor: which just confirms what we had before for our CH three for that first peak. Then for a second peak at 4.1,

00:14:05:32 - 00:14:11:48
Instructor: integrates for two, most likely being a CH two. For the last peak, integrates for one.

00:14:11:48 - 00:14:27:15
Instructor: Mine is just one hydrogen from our carboxylic acid. And for the last item in our list is splitting.

00:14:27:15 - 00:14:36:47
Instructor: We can see that the first peak splits as a triplet, meaning it has two other hydrogens around it. For the second peak at 4.1,

00:14:36:47 - 00:14:48:99
Instructor: it splits as a quartet, meaning it has three neighboring hydrogens and for the last peak is a singlet, meaning no neighboring hydrogens. So your last.

00:14:52:83 - 00:15:14:63
Instructor: Now that we have all of our pieces together and the splitting so we know how they connect, we can put our molecule together, starting with the carboxylic acid, which always goes at the end. Knowing the rules that the oxygen makes it go more downfield, we do expect our CH two to be the closest one and next to the oxygen.

00:15:14:87 - 00:15:31:79
Instructor: Then finishing off with our CH three. Now taking a look at our molecule all complete, we can look that this CH two splits as a quartet because of three neighboring hydrogens and the CH three splits as a triplet because of the CH two.

00:15:31:79 - 00:15:48:01
Instructor: Notice that the singlet it's not close to any other neighboring hydrogens and shows up in the spectrum. Taking a look at this example, we have a little bit of a more complicated spectra in this molecular formula.

00:15:48:01 - 00:15:55:17
Instructor: The first item in our list, we can count the peaks. Look, there's four peaks, meaning four different environments.

00:15:55:17 - 00:16:04:13
Instructor: Now, noticing that first peak showing a 2.3 PPM, which is most likely a CH three, and that peak at 3.8 is a little bit more downfield,

00:16:04:13 - 00:16:07:87
Instructor: so that's something to keep in mind. Now taking a look at the 7.0 region,

00:16:07:87 - 00:16:42:31
Instructor: we have two distinct peaks, meaning there's two things happening in the aromatic region. Now, look at number two for any electron withdrawing group, we do have an oxygen which will make any peaks go more downfield, and we just noticed that at 3.8 is a little bit more downfield than normal,

00:16:42:31 - 00:17:01:22

Instructor: which is most likely close to the oxygen. Then for our third item, we look for integration, knowing that our first peak integrates for three, most likely a CH three, and then the peak at 3.8 also integrates for three,

00:17:01:22 - 00:17:07:08
Instructor: which most likely another CH three. Then for aromatic peaks, they both integrate for two.

00:17:07:08 - 00:17:21:49
Instructor: However, we have two distinct groups of two hydrogens each. Now taking a look at number four for splitting.

00:17:21:49 - 00:17:37:73
Instructor: Our first two peaks are singlets, meaning they don't have any neighboring hydrogens around it. And our peaks in the aromatic both split as a doublet, meaning they fill itself plus one neighboring hydrogen.

00:17:44:25 - 00:17:59:55
Instructor: Now that we have all of our pieces, we can put them together, always starting by the aromatic molecule. Now that we have our aromatic ring, then we can start placing our CH three in a way to maintain symmetry.

00:17:59:55 - 00:18:08:41
Instructor: By doing that, we have two sets of equivalent hydrogens. Now I'm placing them opposite of each other to maintain that symmetry.

00:18:09:05 - 00:18:17:61
Instructor: I'm leaving it blank just because we still have an O to deal with. Remember that a 3.8 peak is equivalent to a CH three,

00:18:17:61 - 00:18:31:85
Instructor: it's a lot more downfield than normal, meaning it's most likely closer to the oxygen. In this case, knowing that everything remaining in our ring is those two set of hydrogens, the oxygen must go in those places of the R groups.

00:18:32:49 - 00:18:40:23
Instructor: Now we only have the two remaining sets of hydrogens to place. Knowing that the peak at 7.0 is more downfield,

00:18:40:23 - 00:18:51:60
Instructor: we do expect to be closer to the O. Now that we have our molecule all complete, we can double check the splitting.

00:18:51:60 - 00:18:55:52
Instructor: We know that HB feels HA. That's why it splits as a doublet.

00:18:55:52 - 00:19:16:84

Instructor: Same thing with HA, which feels HB and it splits as a doublet and HB is a bit more downfield because it's closer to the out, just like the two CH threes that are singlet because they're not close enough to any of other hydrogens. Now after going through it, for any spectra that you get, you can follow those four steps and you should be able to solve it.