So today I'm going to begin talking you through how to interpret a 1D NMR spectra software I've used today is by broker topspin, and you can download this from their website. You can also obtain a free academic licenses. Also, along with the software download. It's the purpose of today not to describe exactly with all the buttons of Topspin do. Here is just to show you how to interpret a basic interpretation of an NMR spectrum. Here we have a 1D NMR spectra. So NMR traditionally for the 1D tends to run from about 0 PPM all the way up. So about 12 PPM. And the spectrum of a zoom out, you can see that the scale goes all the way up to extending about 15 ppm. So what do we start looking at? Where we start looking at spectra? So just having a look here, our spectrum, we can see that left hand side is occupied by a number of peaks. Peaks present in the middle of the spectrum, and their peaked present also at the right-hand side. Well, it's one of the first things we look at when deducing what it is that we have. Well, we need to make sure, is this just one thing in our sample or not? How do we determine this? Well, we can have a gauge based on by just simply looking at the spectra to look all the different peaks. Are some of them the same height or some of them not the same height. We can also get an indication of the integration, for example, at the bottom, to see what integration either matches or it doesn't match. Here you can actually see just by visually seeing that there is a region over towards the right hand side and the aliphatic region of the spectrum where there appears to be some form of impurity peaks or perhaps even a compact. However, because the sample was run in chloroform. So you can see here deuterated chloroform shoes. Chloroform traditionally comes about 7.26.9 ppm. And every time you run a sample, you tend to always gain, get the presence of water signal. And this year would be indicative of the water signaled as President chloroform. So the sample, just by looking at it, they will be deemed was probable impurities as actually come from using the solvent itself. Therefore, the sample looks to be relatively clean. So how do we start interpretative spectra? For me, I always tend to look at the left-hand side to the spectra because it's the easiest types of spectra to look up. And why is that? Aromatic peaks tend to run from 69 ppm. Aromatic carbons can only contain one hydrogen atom at any one time. Which means that in this region, a single peak should infinity by white just said, gives off one hydrogen atom. However, you can see here that the integration doesn't quite match it saying that there's 3.53 protons and buy based on why just said, this is not possible because a carbon atom in this region cannot contain three hydrogens. So therefore, what we say is, okay, let's take a look and see what we've got. So zooming into the spectrum, we can see that we have two nice sets of doublets and they're separated by quite a distinctive ppm. We want to try and deal with this integration farce. We need to figure out, well how many protons in their sample RB dealing with. So let's start to manipulate the integration. We want to say based on what I said, that the aromatic peak is equivalent to one photon. And here you can see there's a nice correlation between these two peaks, which means the pair of these add up together. So it looks like that we do have two aromatic peaks. But what we must do as B must then take a look and say, well, what's the best of the sample look like. You can see here by looking toward the middle on the right hand side that the spectra that we have here, we've got a peak here that is correlated to half a proton, maybe can't get half a proton. And there was this something an impurity or is actually related to our sample. We look again at this nice singlet here and we can see, well actually here it says there's 1.6 of a proton. And again, this is not possible. Which means by looking just at these three additional peaks, we can say that we've actually picked the wrong integration for the aromatic region. Way kinematic peaks b, a greater than one, or when you have equivalent protons. In this particular case, why don't we say that we actually have a potential of equivalent protons and let say this value could potentially be too. You can see here again a nice correlation between these two. And then if we zoom up to time, take a look at the rest of the peaks, we can now see that this peak that was once a half, that integrates to one, this peak that was 1.6 million degrees to 30. So it does actually look like we pick the wrong integration for the aromatic region. But we now know that this peak, this sample now has four aromatic protons. So let's take a little look at these aromatic

protons. By zooming in. We can see that they are doublets, but they do contain fetish small a coupling. Well, suggesting potential long-range coupling. However, nonetheless, let's pay attention to the biggest complaint, which is the fact that they're splitting as a doublet. The fact that they are both even, and it's telling you that there are equivalent protons, which means the set of protons has one neighbor, correct? Which means on its other sites, there must be a substituent. So what we can do now is let's take a look at the structure editor and we're going to pick just the most simplest of aromatics to begin with, which is the benzene ring. Let's look at this. From here now. We are wanting to say a single proton. So let's let this proton, and we said that it had exactly one neighbor. So let's draw n. This one neighbor, QD is here, and he splits off now and feeding into a doublet. Fine. However, what is present on his other sites, remember, we're talking about that. That means that it must be substituent and disposition here. So for the sake girl, let's draw it in. So here is a substituent here. So, so far we've been able to identify this is what at least potentially one site of that red looks like. Going back to the spectrum, let's take a look at the other peak. The other peak is near identical. It has the same doublet pattern as well, suggesting that it has the same sort of substitution. So going back to the structure editor, we then start to say, OK, let's draw this same typologies. Let's draw it in the same. And we see here there's one hydrogen, has one hydrogen neighbor. And again, there must be another substituent. So here we draw the substituent located in this place. Yeah. So the fact that integrates a doublet, it has one neighbor. The fact is whether there's long-range coupling suggests the potential for to see something else. Okay. So this here would be indicative of a powder substitution. Looking at these peaks in the spectrum is suggesting to you that is part of substitution. You have two sets of equivalent protons, each separated by reasonable ppm. Now let's take a look at the end of the spectrum. Let's take look at the middle. So we have three peaks that we have to assign. We have a very broad here. We have a nice tall sharp singlet here, and we have a doublet here. So actually, let's take a look at all three of these speaks at once. So traditionally in the NMR, aliphatic peak run from the region of 0 to three PPM. Now as something aliphatic moves closer to the end of its region, as in this case would be indicative of three. It suggests it's a light next to something that's electronegative. Something that is pulling the electron density from this hydrogen atom and moving it further and further away from its desired region. Anything that is deemed coming outside of its region. So it means it comes above three and is still aliphatic, means it must be next to something incredibly electronegative to have effectively D, shielded or stripped away its electron density. The fact here by taking a look at this peak is our nice doublet suggests to you then that this peak must have a neighbor of one. Zooming back out again, let's have a look at the spectrum. So if this has a neighboring one, We then like to take a look at what, where does it fall in the NMR spectrum. You can see here that if this peak is indeed aliphatic, so this can be alkene or alkyne. You can see that it's moving up closer to three, which means it must be next to something electronegative, so it's not connected onto another aliphatic. We look here, we see that this peak integrates to three. Now is it three single protons or is a CH3? And this particular case, we will assume that this is a CH3 because of its nice splitting pattern, splits off into a nice doublet. So going back to our structure editor, we're then going to start to draw on what we know. We know that we have a CH3 and we know that the CH3 is connected onto something electronegative. That's something we do not currently know. We do know, however, based upon it's splitting pattern with this CHD, but it's a doublet. But she suggests to you it has one neighbor. Could, all these one neighbors B? Well, the one neighbor could potentially be. So lets just start to draw these in. We could potentially have an OH, as a neighbor, navigate, the hydrogen on the oxygen is one, and it would therefore then splits this peak into two. So this makes sense to us here, behalf methanol. We can then draw an another peak. We can say, okay, the next potential, if it is a hetero Latin or something electronegative, we can say that its nitrogen an NH2. However, this NH2 would split this peak into three. So it's not an NH2. But what happens if it was an NH? So what we can do is we will then draw n. Oops, my

mistake. We will end draw this and say that it's got connection. We can therefore maybe say, okay, maybe this CH3 is connected onto an NH. So this splitting totally matches. But now we need to see what could this then? And each B, it must be connected onto something, must have something substance substituted and its place. So differentiating between these two, we are looking to try and eliminate what could it be or what could it not be. So we look back and we say, okay, we know that this sample contains one compound. All of our integrations add up quite nicely. Taking a look and we say, Well, it definitely can't be methanol then, because that would therefore be the end of the sample, it would suggest to you that you have a compound pluses. Well, you have this methanol peak. You have these methanol peaks sauteing methanol, so lightened the references associated with us. You can have a look in the solvents table and you can see that this is not the chemical shifts that methanol, traditionally Pearson and chloroform. So it's again, it's giving you extra evidence that it's not methanol. So therefore we say, okay, so far it looks like the potential that citizen nitrogen species aren't as well, could also be an SH. Just depends. So let me draw that in as well. Let's say that we also have ourselves the SH. So we will draw the sulfur atom. However, like you can say again, just the same as, as with methanol. If we were to draw a substituent onto here because we knew if have 11 molecule in the sample, that is therefore the substitution that is there for the compound over. So therefore it's not self-harm. So already just by looking at just at the peak shape and as well as when it falls in ppm, we've already managed to exclude two electronegative elements, the oxygen and the sulfur for being a substituent. This CHD was connected onto. As we are evident here. If it is connected onto a heteroatoms, we should also see this peak here. Now hetro atoms tend to fall within the vision of 32x. And again, the same rules apply. Whatever is connected onto, deeming it being more electronegative, the farther up the spectra it moves, as it moved closer towards sex to the end of its region. Looking here, we see another two potential peaks that we can select from. Here, we see a nice broad peak located at about 4.2 PPM. Abroad peak is often indicated that it is a hetero atom in place. And these broad peaks I often calls fat and lazy. These heteroatoms often appear as bots and lazy. So when you see an a spectra, this sort of peak, you're often telling you that you have the potential of an OH or an SH in your sample dependent on the chemical structure. If you have a hetero atoms, sometimes it can also split into nice distinctive peaks. But most often this is healthy, can appear. So potentially, maybe this peak is associated with this peak. How would it be able to tell? Well, this will be explained in later talks using 2D NMR analysis. For now goes looking at this. If this is a hetero atom, is telling us that there's only one proton associated with this there for when we look back to our structure is giving us indication that best if it is an NH is connected on to something else, it has to be an H connected onto this methyl. What is this N H connected onto? But so far we don't know, but based because we've got an aromatic system and we know we have two substituents. Potentially it could be one of these substituents because remember, the nitrogen atom doesn't look like it's seeing anything else, but it's really hard to tell because it's a broad peak. So for now, why don't we just assume that one of these substitutions onto this ring is an actual fact. This NH methyl. Taking a look back at the spectrum, again, we have one peak left anolytes. And here we have a nice single. Singlets again are and dictate that it contains no neighbors. Hence, y appears as a singlet. The region in the spectra of falls in is either a hetero atom or it's falling as an aliphatic that has moved outside its region. And if it isn't aliphatic, why hasn't moved upside which region? What is it next to? What is pulling electrons away from it? The fact that integrates to three is giving us an indication because all of these protons are equivalent that perhaps are connected on to the same carbon atom. Giving us evidence that this looks like to be a CH3. Because this peak falls about 3.9 ppm and looks to be a CH3 is telling us that it's an extra, something incredibly electronegative for not only to reached to the end of its region of three, but it's actually stepped outside of up to 3.8. Going back to the structure as it turned out, now we are interested to say, okay, what all are the possibilities? So just removing this so we have more room to draw it. We're then

going to look at the possibilities of this CH3. So we begin with our first CH3 and we can say, Okay, next to something incredibly electronegative. So we can say electronegative species is oxygen. And remember this Oxygen, oops, put infinity, be connected on to something because the CHD contains no neighbors. So perhaps this connecting point here is what's connected onto the rank. Again, one possibility. Looking again. Let's then say, okay, well, other electronegative species can be sent called. So something else is quite electronegative that contains also no neighbors as perhaps a carbonyl species. So from here, we can draw ourselves a carbonyl. Here we have drawn the functional group. So again, the CHD does continue neighbours. It has a connecting point which is fine. And it contains the pulling power of elect. Electronic activity from this group means that this is quite d shielded and it would move outside of its region and up into the next. Let's also think more of the Carbonell species here. And we can say, okay, instead of just looking at a ketone, could it potentially be on aldehyde? However, could be an aldehyde because that would then be the end of the molecule. So let's think again. Let's start to look more into carbonyl species and say, OK, what happens if it's estar What happens if it's an ester? Again, this is possible. What happens again if we say Tierra bash the SDR, so for instances a methyl ester. So again, we can draw this structure and for us again. So here I'm drawing in over Esther. And here is the ester. So gain the CH3 is not Connect, doesn't have any neighbors, is connected onto something electronegative and the pooling power of this carbonyl. And here we can see the attachment point. Okay? We could also say that it's also an MIT, but why was it not being a might? Well, for the same reasons as we said previously. So if we were to draw that right here, we can draw ourselves. This game might forgive me for the lack of artistic minus. What we can say here is our species now can eat that a car just like the SR and this configuration or this configuration. But for this instance, I'm just going to draw and the one here we have ourselves a mite. So if it was our aim might, we should be able to see the NH peak in our spectra, but we don't have any other pieces select from alsos around this particular case. This n h would then split this into two peaks, which is not the case because we have a nice singlet. So what happens if the NH is kept as something else on it? Again, possible, but we don't have any other peaks to select from. If we were looking at this in the reverse order, where the nitrogen was present on the other side, again would be true. And we do not have any more peaks in the spectrum to choose from. So we can start to say, okay, it's definitely not the might. And so now we have the possibility of potentially three different, four different sorting can account for different molecules that can be attached on. We have the two stars, we have the ketone, and we also have the methoxy group. So let's look again back as our spectrum. We now want to pay more attention to these are LaTex, the aromatics are now giving us a hint telling us sort of what is potentially connected onto this room. Look at how big the cup, the distance between these two peaks are that incredibly different. One is more closer to the higher entropy aromatic region here, 7.9. And here we have something much lower down, 6.56.6 PPM. It's an aromatic ring, contains a substituent that says electron donating. Their not possession that is affected by that group would appear further down the spectrum as in closer to sex. If something was electron withdrawing and effects that position, you could see it start to move up and up as region closer to the higher end of nine ppm. By looking at these two, we can tell that the region or their environment to which this set of protons are exposed to, means that it has something that is giving electrons or giving electrons in comparison to this proton. So there's something potentially electron donating that's affecting these protons. Where does looking at this one here in comparison to the other peak it seeing has something electron withdrawing. There's affecting these possessions. So let's take a look again at our structure. We had already deemed that it looked potential that the NH can connect itself onto the rank. Providing us with the NH micelle drip. The nitrogen is an electron donating species, which means it feeds electrons into the rank and drinks or effects that he possessions on the ring and affects the ortho and affects the product position. We know looking at the peak shapes, the aromatic region, we have a pod of substitution renamed that this region is not affected or is not evidence

in the NMR. Therefore, the ortho positions are the ortho position. Therefore, because of this electron donating group, would therefore appear closer to six, which we do have that in our, in our spectra. Looking out at the other two remaining peaks, based on what we had said previous, buy them falling closer up towards eight ppm. Looking at it, we can say OK, there's something that's electron withdrawing that is located in this position here that is affecting these electron withdrawing effect. Again, the ortho and the powder positions. Looking at our range, our selection, we can therefore automatically rule out
the methoxy group. The methoxy group is an electron donating species to the rank. So therefore, we can remove this from our selection. We therefore, authorities do not know why flip up. Therefore, we have the option now of three, we have the Kissel. I'll be happy to, to Esther derivatives here. Which one could it be? Well, looking from the spectrum, we know that its inlet next to something electron withdrawing. We know that f has no neighbors and we ignore that the aromatic peaks are telling us that there's an electron withdrawing substituent directly attached onto that ring, which therefore means the connection of the structure. Remember these are the connecting bonds connecting it to the ring. Here, the oxygen is effectively donating to the rain or partially donating. So what we can say is this configuration of the ester is not sufficient for our claim. And we say, okay, we are left with two of these species. Based on in-house knowledge or based on the more, more spectra that you do is this S star that is connected, sharon. So what we have here is we have ourselves the Carbonell and we have ourselves the methyl ester. That's based upon knowledge of looking at spectra, that is where that peak falls in this region is evident. That looks to be like an I start this connected onto. However, if you have more tools available to you, for instance, like LCMS you build to get molecular weight for this compound and each soon be able to deduce, deduce, sorry the difference between these two compounds. Additionally as well, you can also use NMR methods as well. Some 2D experiments can help you say if this CH3 is next to the carbonyl group, or for instance, the CH3 can't see the carbonyl group. And again, these will be explained and laser talks. So by simply deducing all the different regions of the spectrum are very simple spectrum, but nonetheless still provides itself with challenges. We have been able to therefore identify that this compound is part of substitutes. It contains the knee felt Amy as one substituent and also contains the methyl ester and the other. To give us this final compound.

So today I'm going to begin talking you through how to interpret a 1D NMR spectra software I've used today is by broker topspin, and you can download this from their website. You can also obtain a free academic licenses. Also, along with the software download. It's the purpose of today not to describe exactly with all the buttons of Topspin do. Here is just to show you how to interpret a basic interpretation of an NMR spectrum. Here we have a 1D NMR spectra. So NMR traditionally for the 1D tends to run from about 0 PPM all the way up. So about 12 PPM. And the spectrum of a zoom out, you can see that the scale goes all the way up to extending about 15 ppm. So what do we start looking at? Where we start looking at spectra? So just having a look here, our spectrum, we can see that left hand side is occupied by a number of peaks. Peaks present in the middle of the spectrum, and their peaked present also at the right-hand side. Well, it's one of the first things we look at when deducing what it is that we have. Well, we need to make sure, is this just one thing in our sample or not? How do we determine this? Well, we can have a gauge based on by just simply looking at the spectra to look all the different peaks. Are some of them the same height or some of them not the same height. We can also get an indication of the integration, for example, at the bottom, to see what integration either matches or it doesn't match. Here you can actually see just by visually seeing that there is a region over towards the right hand side and the aliphatic region of the spectrum where there appears to be some form of impurity peaks or perhaps even a compact. However, because the sample was run in chloroform. So you can see here deuterated chloroform shoes. Chloroform traditionally comes about 7.26.9 ppm. And every time you run a sample, you tend to

always gain, get the presence of water signal. And this year would be indicative of the water signaled as President chloroform. So the sample, just by looking at it, they will be deemed was probable impurities as actually come from using the solvent itself. Therefore, the sample looks to be relatively clean. So how do we start interpretative spectra? For me, I always tend to look at the left-hand side to the spectra because it's the easiest types of spectra to look up. And why is that? Aromatic peaks tend to run from 69 ppm. Aromatic carbons can only contain one hydrogen atom at any one time. Which means that in this region, a single peak should infinity by white just said, gives off one hydrogen atom. However, you can see here that the integration doesn't quite match it saying that there's 3.53 protons and buy based on why just said, this is not possible because a carbon atom in this region cannot contain three hydrogens. So therefore, what we say is, okay, let's take a look and see what we've got. So zooming into the spectrum, we can see that we have two nice sets of doublets and they're separated by quite a distinctive ppm. We want to try and deal with this integration farce. We need to figure out, well how many protons in their sample RB dealing with. So let's start to manipulate the integration. We want to say based on what I said, that the aromatic peak is equivalent to one photon. And here you can see there's a nice correlation between these two peaks, which means the pair of these add up together. So it looks like that we do have two aromatic peaks. But what we must do as B must then take a look and say, well, what's the best of the sample look like. You can see here by looking toward the middle on the right hand side that the spectra that we have here, we've got a peak here that is correlated to half a proton, maybe can't get half a proton. And there was this something an impurity or is actually related to our sample. We look again at this nice singlet here and we can see, well actually here it says there's 1.6 of a proton. And again, this is not possible. Which means by looking just at these three additional peaks, we can say that we've actually picked the wrong integration for the aromatic region. Way kinematic peaks b, a greater than one, or when you have equivalent protons. In this particular case, why don't we say that we actually have a potential of equivalent protons and let say this value could potentially be too. You can see here again a nice correlation between these two. And then if we zoom up to time, take a look at the rest of the peaks, we can now see that this peak that was once a half, that integrates to one, this peak that was 1.6 million degrees to 30. So it does actually look like we pick the wrong integration for the aromatic region. But we now know that this peak, this sample now has four aromatic protons. So let's take a little look at these aromatic protons. By zooming in. We can see that they are doublets, but they do contain fetish small a coupling. Well, suggesting potential long-range coupling. However, nonetheless, let's pay attention to the biggest complaint, which is the fact that they're splitting as a doublet. The fact that they are both even, and it's telling you that there are equivalent protons, which means the set of protons has one neighbor, correct? Which means on its other sites, there must be a substituent. So what we can do now is let's take a look at the structure editor and we're going to pick just the most simplest of aromatics to begin with, which is the benzene ring.

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However, what is present on his other sites, remember, we're talking about that. That means that it must be substituent and disposition here. So for the sake girl, let's draw it in. So here is a substituent here. So, so far we've been able to identify this is what at least potentially one site of that red looks like. Going back to the spectrum, let's take a look at the other peak. The other peak is near identical. It has the same doublet pattern as well, suggesting that it has the same sort of substitution. So going back to the structure editor, we then start to say, OK, let's draw this same typologies. Let's draw it in the same. And we see here

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