Quantitative Methods in Chemistry

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Lecture – 47
Course Revision

Welcome to the last week of lectures in the course quantitative methods in chemistry. We started this course with an idea of detailing various methods that are present in order to understand, analyze different aspects that one encounters in the field of chemistry and biochemistry and we had set the lectures out in a way where we would build up towards the final week where we would have demos.

Unfortunately, due to the Coronavirus situation, we cannot record demos right now so therefore we are resorting to the (()) (1:00) mode where we will be revising what we have done in the first 11 weeks. So even before we go towards the revision I and Aasheesh would like to quickly summarize what is that we wanted to do for this demo so that at least that part becomes a little clear.

So what I wanted to do was that since we have learnt how to numerically simulate, understand quantify errors, standard deviation, variance. So what I wanted to do was to take an enzyme and then perform Michaelis-Menten kinetics, give the kinetic rate profile where from that you will be plotting the velocity of reaction as a function of concentration of the substrate.

And then be able to understand yourself how to repeat help, where do standard deviations and how do systematic errors come up, how do random errors come up, where do fluctuations come from all this was actually the idea and finally taking it towards data fitting where one would be able to use this data in order to understand and apply the concepts that Aasheesh introduced in fourth and fifth week of how to analyze the data towards okay what is right, what is not right and how to identify outliers and all that.

So that was one of the significant part that was thought of where we would be shooting on how samples are prepared, how concentrations are estimated for a protein using UV-visible spectrophotometry and then following an enzyme kinetic assay using the same methodology

Unfortunately, this did not go through, but after this we also have plans of how to use the different techniques of let us say chromatography and NMR spectroscopy in order to identify components and delineate them. I will leave it to Aasheesh to explain what ideas we have.

So I think thanks Bharathwaj the plan for us was that apart from what Dr. Bharathwaj has said we will also show you how we undertake a high performance liquid chromatographic separation of compounds, 2 compounds which will be chemically very different for example, something like naphthalene and say naphthol in which case the phenolic (()) (03:08) naphthol will instantiate a very different chemical profile and property.

So we would have shown you practically how this compound or this mixture of compounds is injected into a chromatographic column, chromatographic system rather and then how does it elude through the solvent flow and what kind of detectors we can use and we could have seen in reality the illusion profile of these 2 compounds. We would have ourselves calculated retention times, the width at the base.

And from these numbers we could have easily estimated the plate height and the plate count for the separation that we could have undertaken. Similarly, we could have also undertaken two compounds which are chemically quite similar, but are indeed isomers of each other say we could have taken something like beta-naphthol and alpha-naphthol as our test molecules and could have attempted resolution of these 2 again through chromatographic separation using high performance liquid chromatography.

To demonstrate to you how powerful this chromatographic techniques are and often times how short times are required to achieve high resolutions and separation of the compounds and isolating them in an analytically pure manner and the analytical purity could have been estimate either through UV-Vis spectroscopy or better through NMR spectroscopy of the material that we isolated.

So for that purpose we would have required what is known as a preparative chromatography or prep HPLC as the short form goals where the column thickness is much higher or it is a much thicker column that is utilized. So that we can inject a large amount of material into the HPLC and we can obtain enough quantities to undertake chemical characterization of the material that is purified through this chromatographic technique.

So I guess this was the idea, but at least what we could have we could achieve in this 11 weeks is to cover the theoretical topics in as much detail as we wanted to and I hope this has given you enough incentive to undertake your own analysis of the data that you would generate and we have also attempted to keep the discussion as general and as daily life as possible.

For example, the data that you generate could be a chemical data, could be from physics, from statistical analysis that we perform again, any kind of experimental observation that we repeatedly perform would be analyzed through the statistical tools that were made available to you in this course. So we hope that you take all the concepts forward and apply it in your classes or even in the experiments that you would end up performing.

So therefore now the final result to just revising the last 11 week of lecture starting from my first week. So what I would also want to emphasize here is to keep into mind the idea of significant figures when you are reporting your own data, how the error propagates and what you can do to minimize the error propagation and how those should be incorporated when you are reporting your own data. So now Bharathwaj can summarize the topics that were covered in the first 3 weeks of the lecture. Thank you.