

POINT OF VIEW

Decomartmentalized Knowledge and Core Analytical Chemistry Concepts

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One of the most important skills a researcher can wish for is the ability to take knowledge from one field and seemingly apply it to another. In fact, this is true for researchers and for everyone else. If you keep an open mind, experiences from different periods of your life may be successfully used to solve a difficult problem, even if these (your experiences and the problem at hand) seem totally unrelated at first. I will use an event from my own life as an example (even though it is not a scientific one). Different from other adults driving for the first time on ice/snow, I had no trouble doing it. All because of my teenage years' experience driving my father's VW Beetle (Fusca) in slippery mud. In this spirit, think about how much of the knowledge used to create everything, from planes to computers, comes from different fields. This type of decompartmentalized, unprejudiced approach has always been a powerful force driving scientific and human progress.

As another example of a decompartmentalized approach for solving problems, several recent studies in the biomedical field describe the use of machine learning tools helping researchers better understand gene expression and disease progression, as well as facilitating the development of alternative diagnosis and treatment methods [1,2]. On the other hand, as an atomic spectrometry researcher, I feel elemental information is missing in such studies and could significantly contribute to a more complete overview of medical conditions [3]. As analytical chemists, we could also intensify our collaborations with other fields and offer a unique, specialized perspective on their issues, and at the same time expand the capabilities of our own methods. I know collaborations take time and effort to flourish, particularly because each field has its own interests and its own timeline. However, collaborations are long-term investments for all parties involved. It takes patience, but it is worth it.

In the biomedical field, for example, there are many opportunities for collaboration. Atomic spectrometry researchers are well positioned in this case, as only a relatively small number of studies involving trace element analysis and medical conditions have been reported. In such collaborations, one has the chance to learn and apply new tools, such as supervised and unsupervised machine learning. In combination with the simultaneous multi-element instrumentation available to spectroscopists, these tools allow for developing powerful methods. In addition, with new tools in hand (and keeping an open mind), we can revisit some old problems. Machine learning may help, for example, identify and minimize matrix effects [4], or facilitate the selection of internal standards [5]. There are numerous machine learning techniques that could significantly expand the application of our methods. From unsupervised approaches, such as *t*-distributed stochastic neighbor embedding (*t*-SNE) and uniform manifold approximation and projection (UMAP), to efficient supervised techniques, such as neural networks, support vector machines and random forests. The list is long, and is growing everyday with increased interest for applications in every field. However, as in other areas of life, one has to use a new tool with caution so it produces the desired results. These techniques are as good as the data one feeds them. Therefore, solid analytical chemistry concepts should guide their use, not the other way around.

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To finalize my “*point of view*” on using knowledge from different fields to solve the most varied problems, I would like to say we should strive to apply some of the core concepts of analytical chemistry during these difficult times we are living today. Just as a single point is incapable of indicating a trend, a single person cannot have all the answers. Let us listen to many voices (as we would collect several data points) before reaching a conclusion. Furthermore, let us not give much weight to extreme positions. Just as outliers (when given much importance significantly skew the data), extreme voices often contribute to inaccurate conclusions.

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