AI INTEGRATION IN FTIR SPECTROSCOPY: ENHANCING QUANTIFICATION, **Daniel Vetter**, Anton Paar GmbH

How can Artificial Intelligence (AI) advance the capabilities of Fourier Transform Infrared (FTIR) spectroscopy? FTIR spectroscopy is known for identifying substances and measuring analytes.

We'll look closely at how AI methods can improve the accuracy of quantification in spectral analysis. We examine Partial Least Squares (PLS) models, a standard tool in FTIR analysis, highlighting both their strengths and limitations. Additionally, we compare PLS models with neural networks, assessing their respective advantages and disadvantages.

The comparison shall provide insights into the effectiveness of each approach. Furthermore, diverse applications of neural networks in FTIR spectroscopy are discussed, extending beyond quantification.

The presentation shall provide a clear examination of how AI methods can refine quantification in FTIR spectroscopy, offering practical insights into the integration of PLS models and neural networks within this scientific field.