




**EXPERT**<sup>™</sup>  
Intelligence

# **Unlock AI for Mass Spectrometry Analysis with Expert Intelligence.**

The Expert Intelligence<sup>™</sup> (EI) platform is an AI-automated App Builder for AI applications that interpret noisy or complex mass spectrometry data. The App Builder removes the cost and complexity of creating AI applications - no AI engineering or additional AI tools are required. Go straight from visualized data to a trained AI network embedded in production software to monitor the quality of inference results.

With EI's proprietary Generative Deep Neural Networks (DNNs), unlock hidden results with minimal data. Experience streamlined workflows and enhanced efficiency with EI's advanced techniques for metadata extraction, automatic visualization, and sophisticated AI algorithms eliminate tedious data processing.



**With EI's proprietary Generative Deep Neural Networks (DNNs),** unlock hidden results with minimal data. Experience streamlined workflows and enhanced efficiency with EI's advanced techniques for metadata extraction, automatic visualization, and sophisticated AI algorithms eliminate tedious data processing.

Your expertise is the key to creating customized AI applications tailored precisely to your needs - without the need for dedicated AI engineering or data science teams. With the EI Data Canvas, domain experts such as chemists or materials scientists, with an AI-assisted interface, directly identify the useful part of a signal. AI-driven discovery will profoundly change mass spectrometry analysis by allowing scientists and engineers to look deeper into data obscured by noise and complexity.

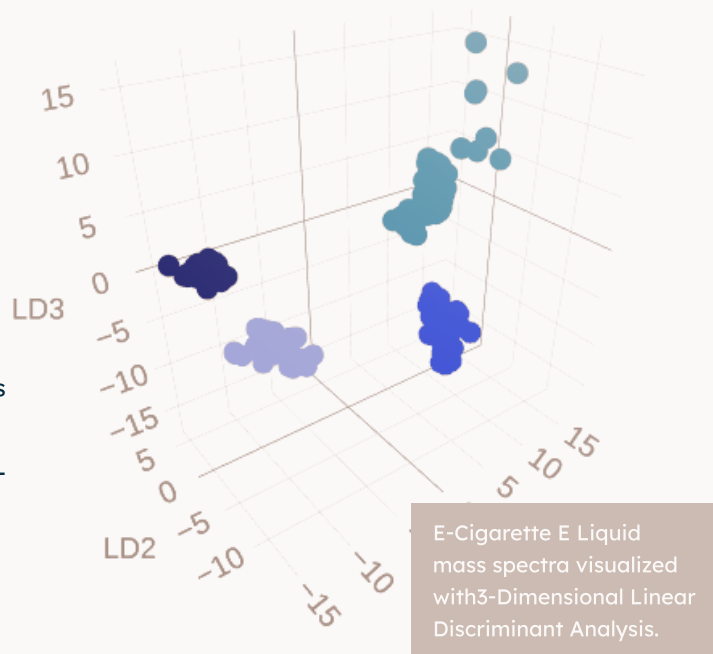
The EI Data Canvas, our intuitive graphical user interface, serves as the gateway to visually navigate and analyze your data. By visualizing mass spectrometry data, a scientist can identify the regions of interest and automatically train a DNN to identify interesting patterns in noisy signal data. AI simplifies the intricacies of mass spectrometry analysis to reveal hidden insights.

In a proof of concept case study focusing on E-cigarettes and E-liquids, EI exceeded all previous methods. Analyzing 48 LCMC mass spectrometry data samples, two EI-generated AI Applications achieved Flavor Profile Classifications with an outstanding accuracy of 98% and Brand Classifications achieved an impressive inference accuracy of 99%. In contrast, prior methods struggled with only 66% accuracy, highlighting the capability of EI in delivering highly accurate and reliable results. In a prior study by Buddenbaum et al. [1] with leave-one-out validation and mixing validation/training subjects achieved 20% and 67% accuracy, respectively.

# In This Case Study, Two Custom AI Applications Were Created With The Automated EI Workflow:

## STEP 1: LOADING THE DATA AND VISUALIZATION

EI's advanced Data Canvas extracts metadata from file names and uploaded content to generate sophisticated visual representations using DNN/ML embeddings. These visualizations enable automatic tSNE, LDA, or PCA visualizations. No manual adjustments required - let the power of AI manage the complexity of your input data.

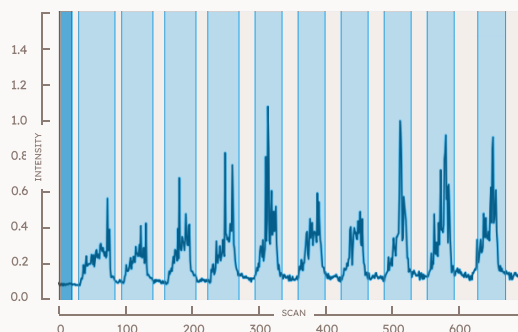


## STEP 2: ANALYSIS SELECTION

EI provided insights into potential applications of the uploaded data, including Brand Categorizations, Flavor Profile Categorizations, Outlier/Anomalous data detection, and Trend Analysis. With AI-assisted guidance on analysis methods tailored to the dataset characteristics, the scientist in the case study quickly pursued multiple avenues of analysis. In this study, two AI Applications were created for Brand Categorization and Flavor Profile Categorization in a matter of days.

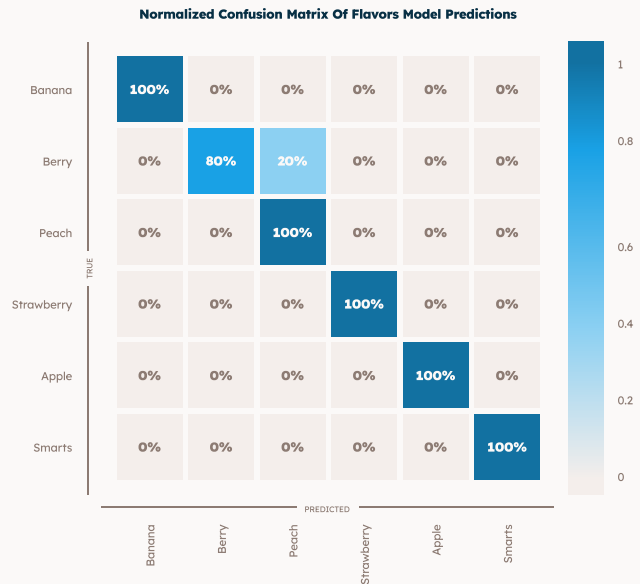
## STEP 3: EXPERT VERIFICATION OF TRAINING

EI's advanced algorithms detected and differentiated spectrums representing the ingested sample (shaded in light blue) and the background (shaded in dark blue/white), showcasing robustness to intensity fluctuations. Furthermore, EI precisely detected multiple regions of interest, even in samples with varying spike peak heights and widths. To assist the process, EI seamlessly integrates your experience and knowledge, leveraging deep learning methods to enhance accuracy.



## STEP 4: BUILD AN AI APPLICATION WITH EI

Building an AI App is supported by embedded AI modules that automate the entire Automate AI engineering process within one environment. Select your data and define critical success criteria. The EI framework then crafts a robust DNN/AI-powered EI App, ready for testing before deployment. Notably, EI App encompasses not only the inference model but also software modules that actively monitor for data drift and concept drifts. The production application also supports active learning on data corrections to dynamically improve accuracy. The EI-generated Flavor Classification App underwent testing using previously unseen data, resulting in a remarkable 100% accuracy on the confusion matrix test for flavor profiles.



## STEP 5: DEPLOY THE AI APPLICATION

Once the model is trained and tested, EI embeds the inference model in a production application that can be accessed through the Expert Intelligence cloud portal. The EI production inference application can also be optionally deployed as a software module for use in analysis software or as an embeddable module.

This example and other case studies have produced extraordinary results. The EI platform is the only AI-powered App Builder that puts experts in control of AI-powered analysis for research, process control, and innovation.



**EXPERT**<sup>™</sup>  
Intelligence

Find Out More  
[expertintelligence.ai](https://expertintelligence.ai)

Experience the limitless possibilities of Expert Intelligence and reshape the future of mass spectrometry analysis. Embrace the power of AI and experience what's possible.