Elsendorf, Bavaria, Germany

# Case Study: Hops

June 2022

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**Contact**

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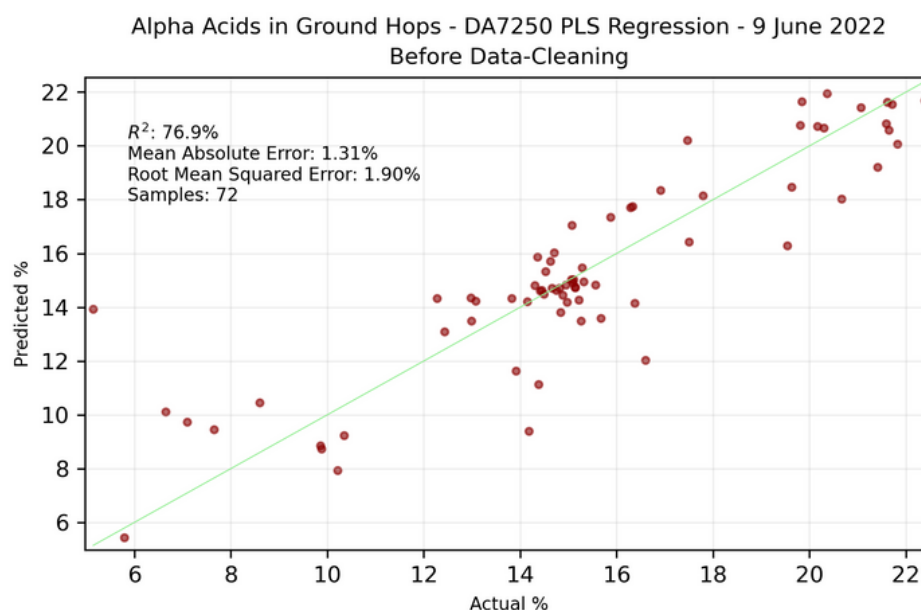
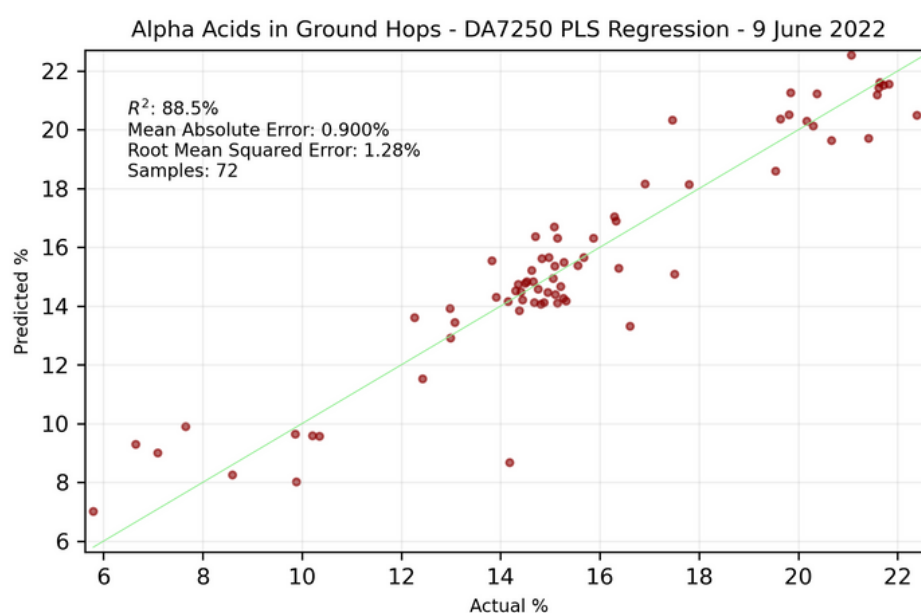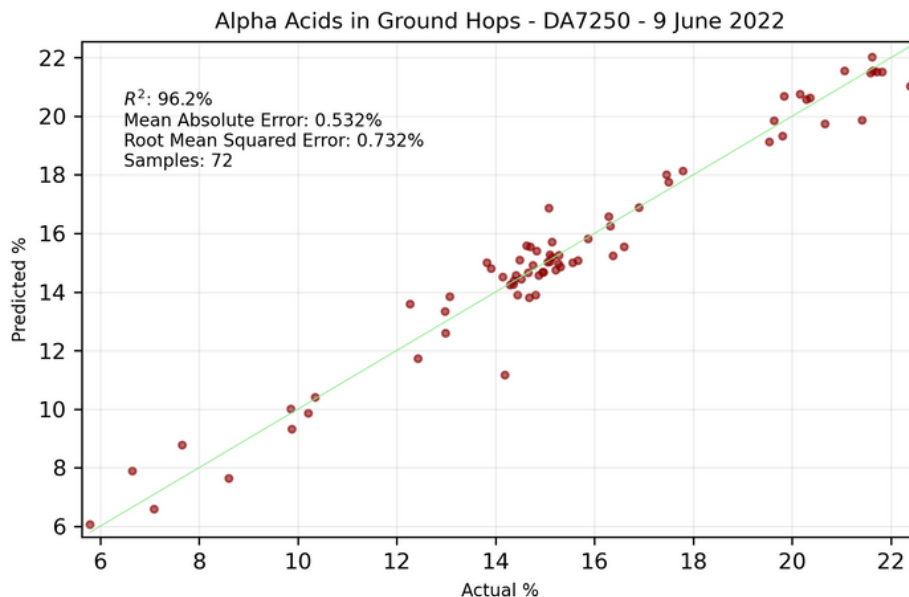📞 +64 21 928 420     ✉ george.hill@sagitto.com     🌐 www.sagitto.com

Sagitto recently developed calibration models for a PerkinElmer DA 7250 at-line NIR instrument, as part of a pre-purchase evaluation exercise conducted by a large hops producer. For the purposes of this case study, we also took the data as supplied and built a calibration model using the widely used Partial Least Squares (PLS) technique, such as is often used with Aspen Unscrambler. This resulted in a model which – on cross validation – had an $R^2$ value of 76.9% and Root Mean Square Error (RMSE) of 1.90%



To illustrate the role that good data cleaning plays in calibration modelling, we then rebuilt the PLS model after applying our usual techniques for data cleaning. This resulted in a model with an $R^2$ of 88.5% and RMSE of 1.28%

By way of comparison, the plot below shows the results after we applied Sagitto's proprietary machine learning techniques to the same cleaned data. Not surprisingly, we were able to generate an even better calibration model using machine learning, with an $R^2$ of 96.2% and RMSE of 0.73%



Alpha Acids in Ground Hops - DA7250 - 9 June 2022

$R^2$: 96.2%
Mean Absolute Error: 0.532%
Root Mean Squared Error: 0.732%
Samples: 72

**Testimonial**

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*With Sagitto's data science service the predictive models are living entities, which allows us to smoothly integrate model maintenance into our calibration system so that the analytical output is of equivalent quality to established brewing industry standard methods of analysis.*

*Sagitto have demonstrated quality, flexibility and awesome turnaround times for model generation and revision.*

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Dr Simon Whittock,
Hop Products Australia