Near Infra-Red Spectroscopy Predicts Crude Protein in Hemp Grain

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Abstract

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**incomplete: may contain errors, run-ons, half-thoughts, etc.**

## 1 INTRODUCTION

Hemp (Cannabis sativa L.) is an annual crop with potential uses as a source of food or feed from grain, and bast fiber or hurd from the stalk. Hemp cultivars are commonly grown for one or both purposes and a cultivar may be referred to as a grain, fiber, or dual-purpose type. Because of protein’s nutritional importance, the protein content of a grain crop is an prime consideration for researchers, producers, and consumers. Whole hemp grain typically contains approximately 20-30% protein (Bárta et al., 2024; Ely & Fike, 2022; **callaway2004?**). Crude protein (CP) is often used as a proxy for the direct measurement of protein concentration and consists of the multiplication of nitrogen concentration by a conversion factor because measuring nitrogen concentration is relatively easy and cheap via laboratory assay (Hayes, 2020).

Near-infrared spectroscopy (NIRS) technology is rapid, non-destructive, and cheap, and consists of the measurement of NIR radiation reflected from a sample (Roberts et al., 2004). NIR spectra from many samples are related to laboratory values for components such as moisture, protein, fat, or fiber (Roberts et al., 2004). NIRS technology has been used since the 1970’s to assess forage CP (Reeves, 2012; Williams, 1975). A NIRS calibration set often consists of samples from one species grown in many environments encompassing the range of expected values from the analyte or analytes (Chadalavada et al., 2022). Partial least squares regression (PLSR) is a typical method used in the agricultural and food sciences to relate spectra to analyte (Roberts et al., 2004). PLSR calculates principal components (PCs) which relate to the dependent variable and summarize the spectra and uses a subset of PCs in order to fit the regression model. PLSR is commonly used in spectroscopy because it tends to work well with highly-correlated spectral data. Typically the number of principal components is chosen via cross-validation to avoid overfitting. **CITES FOR ALL OF THIS**

A NIRS-scanned sample of undamaged grain may used for other purposes or it may planted as a seed. In wheat and corn, grain protein content has been shown to be heritable (Geyer et al., 2022; Giancaspro et al., 2019). This suggests (at least potentially) that NIRS technology could serve as resource to more rapidly identify high CP hemp germplasm, enabling the delivery of higher CP hemp grain cultivars faster.

For this study, a benchtop NIR spectrometer was used to develop a model to predict CP content based on a data set of hemp grain representing multiple years, locations, and cultivars from grain and dual-purpose hemp types using PLSR.

## 2 MATERIALS AND METHODS

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### 2.1 Hemp Grain Sample Background

Spectral data were obtained from whole (unground) hemp grain samples, harvested at maturity, collected from 2017 - 2021 from 18 cultivar trials in New York (NY) (NA samples). Grain samples were obtained by hand sampling or mechanical harvest and were cleaned of chaff and dried at 30 C for six days in a forced-air dryer. In total, 38 cultivars were represented in the data set. Cultivars were grain or dual-purpose types and included both commercially available and experimental material.

All cultivar trials were planted in randomized complete block design with each cultivar replicated four times. The 2017 data were comprised of samples from the same thirteen cultivars sampled from six NY locations. For those trials, grain was harvested from each plot individually and aggregated by cultivar within each trial. Four subsamples were drawn from each aggregated sample and scanned separately. These spectra were averaged at each 2 nm increment. All remaining samples from 2018-2021 were collected on a per-plot basis. All possible cultivars and possible locations were represented in 2017, but only a selected subset of cultivars and locations were represented in 2018-2021.

### 2.2 Spectral Data Collection and Preprocessing

A benchtop NIR spectrometer (FOSS/ NIR FOSS/ NIR Systems model 5000) was used to obtain the spectra (FOSS North America, Eden Prairie, MN, USA). Spectra were collected every 2 nm from 1100-2498 nm and the logarithm of reciprocal reflectance was recorded.

WINISI software version 1.02A (Infrasoft International, Port Matilda, PA, USA) was used to average the spectra in 2017, as well as to select samples for laboratory assay. Samples were selected according to their spectral distance from their nearest neighbor within the calibration data set with a cutoff of a distance of 0.6 H, where H is approximately equal to the squared Mahalanobis distance divided by the number of principal components used in the calculation (Garrido-Varo et al., 2019). Prior to selection selection, spectra were preprocessed using SNV-detrend with settings 1,4,4,1 for the derivative, gap, smooth, and smooth 2 settings respectively.

### 2.3 Laboratory Validation

Laboratory assays were performed by Dairy One Forage Laboratory (Ithaca, NY). For those assays, 1mm ground samples were analyzed by combustion using a CN628 or CN928 Carbon/Nitrogen Determinator. Samples from 2017 were aggregated as described above, but the remaining samples were not aggregated.

### 2.4 Model Development

Calibration and validations sets were created by dividing the laboratory CP values into tertiles according to their percent CP in order to ensure that the range of CP values was present in both calibration and validation sets. Within each tertile, 75% of the samples were randomly assigned to the calibration set and the remaining 25% were assigned to the validation set. For each calibration set, models were developed in caret using PLSR. In fitting the model, the number of principal components was optimized over au grid search from 1-20. Model performance was evaluated with 25 iterations of bootstrapping and minimized root mean squared error (RMSE) in selecting the number of principal components in the final model .

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Initially a number of common spectral preprocessing methods were tested by creating 100 calibration and validation sets as described above. Spectral data from those data sets were transformed by each of the following methods: 1) first derivative, 2) Savitzky-Golay (SG) using the first derivative, third order polynomial, and a window of size 5, 3) gap-segment derivative using the first derivative, a gap of eleven, and a segment size of 5, 4) standard normal variate (SNV), 4) standard normal variate following Savitzky-Golay (SNV-SG) (same SG parameters as above), 5) SNV-detrend with second order polynomial, and 6) multiplicative scatter correction.

For each of these preprocessing methods, models were fit and predictions were made on the corresponding validation set (since there were 8 preprocessing methods, 8 separate models were fit for each of the 100 sets. The relationship between the predicted and actual values of the validation set were calculated via RMSE, R2 and Ratio of Performance to InterQuartile distance (RPIQ), three common model assessment metrics. Larger R2 and RPIQ, and smaller RMSE values are superior. Analyses of variance (ANOVA) were performed for each of these metrics in order to compare the preprocessing methods. For each ANOVA, each data set was considered as a subject and allowing different variances for each preprocessing method.

Once the most promising preprocessing method was identified, 1000 more data sets were created and analyzed via that method and performance on the validation sets was summarized with RMSE, R2, and RPIQ.

### 2.5 Additional software used

We used R version 4.3.3 (R Core Team, 2024) and the following R packages: caret v. 6.0.94 (Kuhn & Max, 2008), data.table v. 1.15.2 (Barrett et al., 2024), emmeans v. 1.10.0 (Lenth, 2024), nlme v. 3.1.163 (J. Pinheiro et al., 2023; J. C. Pinheiro & Bates, 2000), pls v. 2.8.3 (Liland et al., 2023), prospectr v. 0.2.7 (Stevens & Ramirez-Lopez, 2024), skimr v. 2.1.5 (Waring et al., 2022), tidymodels v. 1.1.1 (Kuhn & Wickham, 2020), tidyverse v. 2.0.0 (Wickham et al., 2019).

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## 3 RESULTS AND DISCUSSION

### 3.1 Laboratory assay CP values

Laboratory assay percent CP values are summarized in the following table. These are similar to the range of CP values observed in the literature, indicating an reasonable basis for a chemometric model. The CP values are left-skewed and two thirds of the samples contained more than 25% CP.

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| Table 1: Summary of Laboratory Assayed CP Values (Percent Dry Matter)   | Mean | Sd | Minimum | First Quartile | Median | Third Quartile | Maximum | | --- | --- | --- | --- | --- | --- | --- | | 26.1 | 2.5 | 20.8 | 23.9 | 26.4 | 28.2 | 30.8 | |

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### 3.2 Preprocessing methods comparison

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All preprocessing methods outperformed raw spectral data [Table 2](#tbl-preproc). Averaged together, all preprocessed spectra were superior to raw spectra, with lower RMSE, and higher R2 and RPIQ values (significant at level <0.001). Preprocessing methods had -11.6 % lower RMSE, and had 3.1% higher R2 7.4% higher RPIQ than unprocessed spectra.

The SNV-SG method had the lowest RMSE, highest R2, and highest RPIQ averaging over all iterations. SNV-SG RMSE averaged 1.4% lower, while R2 and RPIQ averaged 0.4% and 2.4% higher respectively than the next best preprocessing method (SG in both cases), but the difference between the best and second best method by metric were only statistically significant at <0.05 for RPIQ. RPIQ was devised to accurately reflect the spread of data in skewed populations (**bellon-maurel2010?**) and thus offers a robust metric for model assessment in this context, where the CP data are skewed. Therefore the superiority of SNV-SG as measured via RPIQ made it the best choice for the final model.

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| Table 2: Evaluation of Preprocessing Methods by Metric ± Standard Error   | Preprocessing Method | RMSE |  | RPIQ | | --- | --- | --- | --- | | Standard Normal Variate following Savitzky-Golay | 1.02 ± 0.012 | 0.84 ± 0.004 | 3.97 ± 0.076 | | Savitzky-Golay | 1.03 ± 0.012 | 0.83 ± 0.004 | 3.88 ± 0.072 | | First Derivative | 1.07 ± 0.013 | 0.82 ± 0.004 | 3.77 ± 0.075 | | Standard Normal Variate | 1.12 ± 0.016 | 0.80 ± 0.005 | 3.61 ± 0.081 | | Gap-segment Derivative | 1.12 ± 0.018 | 0.81 ± 0.006 | 3.60 ± 0.086 | | Standard Normal Variate-Detrend | 1.13 ± 0.015 | 0.80 ± 0.005 | 3.55 ± 0.079 | | Multiplicative Scatter Correction | 1.17 ± 0.016 | 0.79 ± 0.006 | 3.47 ± 0.080 | | Raw Spectra | 1.22 ± 0.044 | 0.79 ± 0.009 | 3.42 ± 0.105 | |

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SNV and SNV-detrend correct light scatter. SG is a smoothing filter that regresses on the signal over a series of windows. Derivatives remove noise, but not necessarily light scattering. **cite**

**cite:** Barnes RJ, Dhanoa MS, Lister SJ. 1989. Standard normal variate transformation and de-trending of near-infrared diffuse reflectance spectra. Applied spectroscopy, 43(5): 772-777.

The preprocessing methods examined represent a portion of those available. As well, preprocessing methods tend to have a number of user-adjustable parameters whose various permutations were not tested. This subset of preprocessing methods and parameters nonetheless contained substantial variations in model quality, demonstrating the importance of the selection of an appropriate preprocessing method.

### 3.3 Final model development and summary

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The model improved most rapidly as the number of principal components increased from 1 to 7, with the inclusion of each additional PC being associated with a decrease in RMSE of 5-12% . From 8 to 12 PCs, model performance continued to improve, although gains were more modest (decrease in RMSE of 0.7-3%). With 13 or more PCs, performance gains were minimal and the relative ranks of the models tended to be stable [Figure 1](#fig-model-calibration).

|  |
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| Figure 1: Decreasing RMSE with increasing number of PCs |

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Final model performance was similar, but not identical to, that obtained during the initial comparison of preprocessing methods. The final models’ mean RMSE was 1.03, R2 was 0.83, and RPIQ was 3.89 (all calculated on the test sets). Despite the generally good model performance, a subset of poor models can be seen. For example, [Figure 2](#fig-final-metric-boxplot) shows twenty-one models with R2 below 0.7. **more comment on poor models?**

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| Figure 2: Final model validation set performance (1000 iterations) |

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Call:  
lm(formula = difference ~ adj\_cp, data = temp\_dat)  
  
Residuals:  
 Min 1Q Median 3Q Max   
-2.51794 -0.58132 0.06936 0.50754 2.74745   
  
Coefficients:  
 Estimate Std. Error t value Pr(>|t|)   
(Intercept) 0.80412 0.17827 4.511 1.31e-05 \*\*\*  
adj\_cp -0.15334 0.03051 -5.026 1.44e-06 \*\*\*  
---  
Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1  
  
Residual standard error: 0.9138 on 147 degrees of freedom  
Multiple R-squared: 0.1466, Adjusted R-squared: 0.1408   
F-statistic: 25.26 on 1 and 147 DF, p-value: 1.438e-06

ith\_in\_data\_set preds crude\_protein cutpoints plot\_order  
 <int> <num> <num> <fctr> <int>  
 1: 50 0.8041160 20.8 (20.8,24.1] 1  
 2: 42 0.7274479 21.3 (20.8,24.1] 2  
 3: 52 0.6967806 21.5 (20.8,24.1] 3  
 4: 83 0.6814470 21.6 (20.8,24.1] 4  
 5: 85 0.6814470 21.6 (20.8,24.1] 5  
 ---   
145: 12 -0.6219116 30.1 (27.5,30.8] 145  
146: 55 -0.6219116 30.1 (27.5,30.8] 146  
147: 117 -0.6372452 30.2 (27.5,30.8] 147  
148: 63 -0.6679125 30.4 (27.5,30.8] 148  
149: 112 -0.7292470 30.8 (27.5,30.8] 149

Source: [Article Notebook](https://rvcrawford.github.io/glowing-system/index.qmd.html)

Finally, the pattern of errors was examined on a per-sample basis. [Figure 3](#fig-validation_set_performance)

|  |
| --- |
| Figure 3: Test set prediction errors on a per-sample basis. Actual sample value set to 0, and samples ranked from least to greatest. |

Source: [Article Notebook](https://rvcrawford.github.io/glowing-system/index.qmd.html)

Errors tend to be lower at higher levels of actual CP

Key: <loc>  
 loc ith\_in\_data\_set crude\_protein difference tmp\_ith adj\_cp  
 <char> <int> <num> <num> <int> <num>  
 1: cnoll 4 27.1 -1.826000348 90 6.3  
 2: free 91 23.1 -1.608410140 24 2.3  
 3: free 100 27.5 0.008386084 100 6.7  
 4: free 103 26.0 -0.095290561 64 5.2  
 5: freev 66 28.3 0.156805468 117 7.5  
 6: freev 69 28.7 0.115415937 128 7.9  
 7: freev 70 27.3 0.123941888 93 6.5  
 8: ithaca 123 25.9 0.137420230 60 5.1  
 9: ithaca 124 23.2 2.325322409 27 2.4  
10: ithaca 125 23.2 2.582685059 25 2.4  
11: ithaca 140 23.5 1.597167816 30 2.7  
12: ithaca 146 28.0 -1.965391942 110 7.2  
13: ithaca 148 26.4 0.145123025 76 5.6  
14: mcg 92 22.7 -0.110406545 20 1.9  
15: mcg 94 28.1 -0.067559276 111 7.3  
16: mcg 121 28.3 -2.434565554 115 7.5  
17: mg4e 28 25.4 0.034158139 53 4.6  
18: mg4e 39 26.1 -0.016921027 66 5.3  
19: mg4l 41 26.4 0.118021909 74 5.6  
20: rn041\_gen 108 27.0 2.600884960 86 6.2  
21: rn041\_gen 109 23.7 -1.980462540 33 2.9  
22: rn041\_gen 110 29.0 -2.495337360 135 8.2  
23: rn041\_gen 111 29.6 -1.777305991 140 8.8  
24: rn041\_gen 113 29.5 0.011781362 139 8.7  
25: rn041\_gen 114 27.7 2.115039075 107 6.9  
26: rnooa 14 29.1 -0.003578789 137 8.3  
27: rnooa 18 23.1 2.020690041 22 2.3  
28: rnooa 19 25.3 -0.110141285 52 4.5  
29: rnooa 25 26.6 -2.603177621 78 5.8  
30: rnooa 26 28.3 -2.034162792 114 7.5  
 loc ith\_in\_data\_set crude\_protein difference tmp\_ith adj\_cp  
 grouping temp\_id harv\_year cultivar type  
 <char> <int> <int> <char> <char>  
 1: worst\_predicted\_10\_pct 32 2017 cfx-1   
 2: worst\_predicted\_10\_pct 111 2018 grandi grain  
 3: best\_predicted\_10pct 128 2019 canda grain  
 4: best\_predicted\_10pct 131 2019 nwg-elite dual  
 5: best\_predicted\_10pct 94 2017 picolo   
 6: best\_predicted\_10pct 97 2017 futura 75   
 7: best\_predicted\_10pct 98 2017 cfx-1   
 8: best\_predicted\_10pct 155 2020 nwg-2730 multistate  
 9: worst\_predicted\_10\_pct 152 2020 futura 75 dual\_replant  
10: worst\_predicted\_10\_pct 156 2020 bialobrzeskie multistate  
11: worst\_predicted\_10\_pct 9 2021 logan c2 exp.  
12: worst\_predicted\_10\_pct 5 2021 crs-1 grain\_dual  
13: best\_predicted\_10pct 10 2021 logan x anka c2 exp.  
14: best\_predicted\_10pct 115 2018 nebraska (feral) dual  
15: best\_predicted\_10pct 113 2018 picolo grain  
16: worst\_predicted\_10\_pct 149 2019 h-51 multistate  
17: best\_predicted\_10pct 56 2017 cfx-2   
18: best\_predicted\_10pct 67 2017 futura 75   
19: best\_predicted\_10pct 69 2017 anka   
20: worst\_predicted\_10\_pct 136 2019 earlina 8 grain  
21: worst\_predicted\_10\_pct 137 2019 katani grain  
22: worst\_predicted\_10\_pct 138 2019 joey grain  
23: worst\_predicted\_10\_pct 139 2019 futura 75 dual  
24: best\_predicted\_10pct 141 2019 h-51 dual  
25: worst\_predicted\_10\_pct 142 2019 hliana dual  
26: best\_predicted\_10pct 42 2017 tygra   
27: worst\_predicted\_10\_pct 46 2017 katani   
28: best\_predicted\_10pct 47 2017 cfx-2   
29: worst\_predicted\_10\_pct 53 2017 cfx-1   
30: worst\_predicted\_10\_pct 54 2017 wojko   
 grouping temp\_id harv\_year cultivar type  
 in\_ny loc2  
 <lgcl> <char>  
 1: TRUE geneva  
 2: TRUE freeville  
 3: TRUE freeville  
 4: TRUE freeville  
 5: TRUE freeville  
 6: TRUE freeville  
 7: TRUE freeville  
 8: TRUE ithaca  
 9: TRUE ithaca  
10: TRUE ithaca  
11: TRUE ithaca  
12: TRUE ithaca  
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16: TRUE ithaca  
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This study is limited in that it represents the creation of one model based upon spectra collected from one machine. NIRS calibrations can be unique to a particular machine, even if the machines compared are of the same model (**Reeves\_2012?**) . As well, the calibration and validation sets are relatively small.

This research showed the promise of the use of NIRS in order to make predictions concerning %CP in hemp grain using PLS. Promising preprocessing methods were identified and a model was validated. Further research could refine the model by including more samples or by examining other predictive methods.

## 4 ACKNOWLEDGMENTS

## 5 SUPPLEMENTAL MATERIAL

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| Table 3: Tally of hemp cultivars and locations. Private cultivars are labeled “cultivar1”, “cultivar2”, etc.   | cultivar2 | chazy | freeville | geneva | ithaca | willsboro | Total | | --- | --- | --- | --- | --- | --- | --- | | altair |  |  |  | 1 |  | 1 | | anka |  | 1 | 3 | 5 | 2 | 11 | | bialobrzeskie |  | 1 | 3 | 4 | 1 | 9 | | canda |  | 1 | 1 | 1 |  | 3 | | cfx-1 |  | 1 | 2 | 5 |  | 8 | | cfx-2 |  | 1 | 2 | 4 |  | 7 | | crs-1 | 1 | 1 | 2 | 5 |  | 9 | | cultivar1 |  | 1 |  |  |  | 1 | | cultivar2 |  |  |  | 1 |  | 1 | | cultivar3 |  |  |  | 1 |  | 1 | | cultivar4 |  |  |  | 1 |  | 1 | | earlina 8 |  |  | 1 |  |  | 1 | | experimental1 |  |  |  | 1 |  | 1 | | experimental2 |  |  |  | 1 |  | 1 | | felina 32 |  | 1 | 2 | 3 |  | 6 | | futura 75 |  | 1 | 3 | 4 |  | 8 | | grandi |  | 3 | 3 | 4 |  | 10 | | h-51 |  |  | 1 | 2 |  | 3 | | han-fn-h |  |  |  | 1 |  | 1 | | han-nw |  |  |  | 1 |  | 1 | | helena |  | 1 |  |  |  | 1 | | henola |  |  |  | 2 |  | 2 | | hlesia |  |  |  | 3 |  | 3 | | hliana |  |  | 1 | 1 |  | 2 | | joey |  | 1 | 1 | 1 |  | 3 | | katani |  | 2 | 3 | 4 |  | 9 | | nebraska (feral) | 1 |  |  | 1 |  | 2 | | pewter river |  | 1 |  |  |  | 1 | | picolo |  | 1 | 2 | 5 |  | 8 | | portugal |  |  | 1 |  |  | 1 | | rocky hemp |  |  | 1 |  |  | 1 | | sterling gold |  |  | 1 |  |  | 1 | | swift | 1 | 1 |  | 1 |  | 3 | | tygra |  | 1 | 3 | 4 |  | 8 | | uso-31 | 2 | 1 | 2 | 4 |  | 9 | | wojko |  | 1 | 3 | 4 |  | 8 | | x-59 |  | 2 |  | 1 |  | 3 | | Total | 5 | 24 | 41 | 76 | 3 | 149 | |

Source: [Article Notebook](https://rvcrawford.github.io/glowing-system/index.qmd.html)

## 6 OPTIONAL SECTIONS

## 7 REFERENCES

## 8 FIGURES AND TABLES

Source: [Article Notebook](https://rvcrawford.github.io/glowing-system/index.qmd.html)

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| Figure 4: Timeline of recent earthquakes on La Palma |

Source: [Article Notebook](https://rvcrawford.github.io/glowing-system/index.qmd.html)

Source: [Article Notebook](https://rvcrawford.github.io/glowing-system/index.qmd.html)

Based on data up to and including 1971, eruptions on La Palma happen every 79.8 years on average.

Studies of the magma systems feeding the volcano, such as (**marrero2019?**), have proposed that there are two main magma reservoirs feeding the Cumbre Vieja volcano; one in the mantle (30-40km depth) which charges and in turn feeds a shallower crustal reservoir (10-20km depth).

Eight eruptions have been recorded since the late 1400s ([Figure 4](#fig-timeline)).

Data and methods are discussed in [Section 9](#sec-data-methods).

Let denote the number of eruptions in a year. Then, can be modeled by a Poisson distribution

where is the rate of eruptions per year. Using [Equation 1](#eq-poisson), the probability of an eruption in the next years can be calculated.

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| Table 4: Recent historic eruptions on La Palma   | Name | Year | | --- | --- | | Current | 2021 | | Teneguía | 1971 | | Nambroque | 1949 | | El Charco | 1712 | | Volcán San Antonio | 1677 | | Volcán San Martin | 1646 | | Tajuya near El Paso | 1585 | | Montaña Quemada | 1492 | |

[Table 4](#tbl-history) summarises the eruptions recorded since the colonization of the islands by Europeans in the late 1400s.

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| Figure 5: Map of La Palma |

La Palma is one of the west most islands in the Volcanic Archipelago of the Canary Islands ([Figure 5](#fig-map)).

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| Figure 6: Locations of earthquakes on La Palma since 2017 |

Source: [Explore Earthquakes](https://rvcrawford.github.io/glowing-system/notebooks/explore-earthquakes-preview.html#cell-fig-spatial-plot)

[Figure 6](#fig-spatial-plot) shows the location of recent Earthquakes on La Palma.

## 9 Data & Methods

## 10 Conclusion

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