Supplementary Materials for…

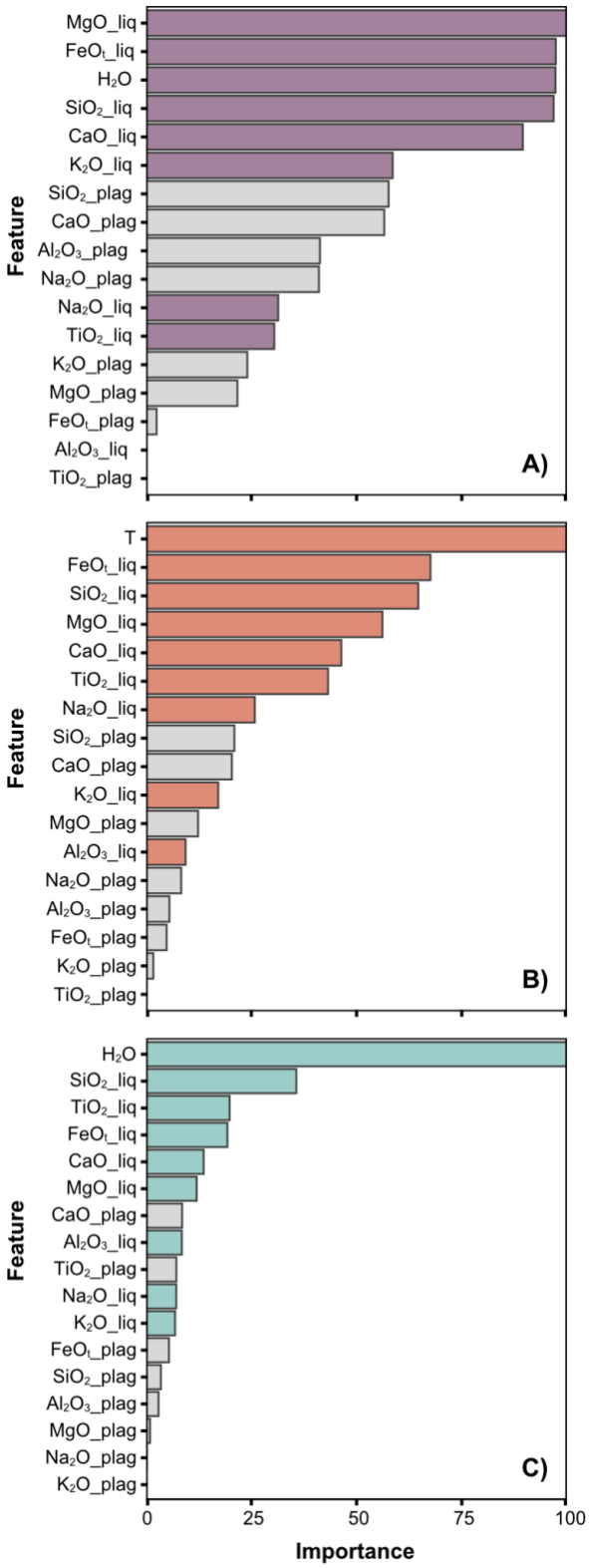
‘Plagioclase-saturated melt hygrothermobarometry and plagioclase-melt equilibria using machine learning’

- **Supplementary Table 1:** Calibration dataset for the thermometers, hygrometers, barometers, and the anorthite content model. *See separate .xlsx spreadsheet.*
- **Supplementary Table 2:** Calibration dataset for the plagioclase-saturated classifier. *See separate .xlsx spreadsheet.*
- **Supplementary Table 3:** Monte Carlo analytical uncertainty simulation input (ten experimental liquid compositions + weighted mean errors of electron microprobe glass oxide analyses) and output. *See separate .xlsx spreadsheet.*
- **Appendix 1:** Error propagation of temperature and water content estimates for hygrometry and barometry (p.2)
- **Supplementary Figures S.1 to S.4** (p.3-6)

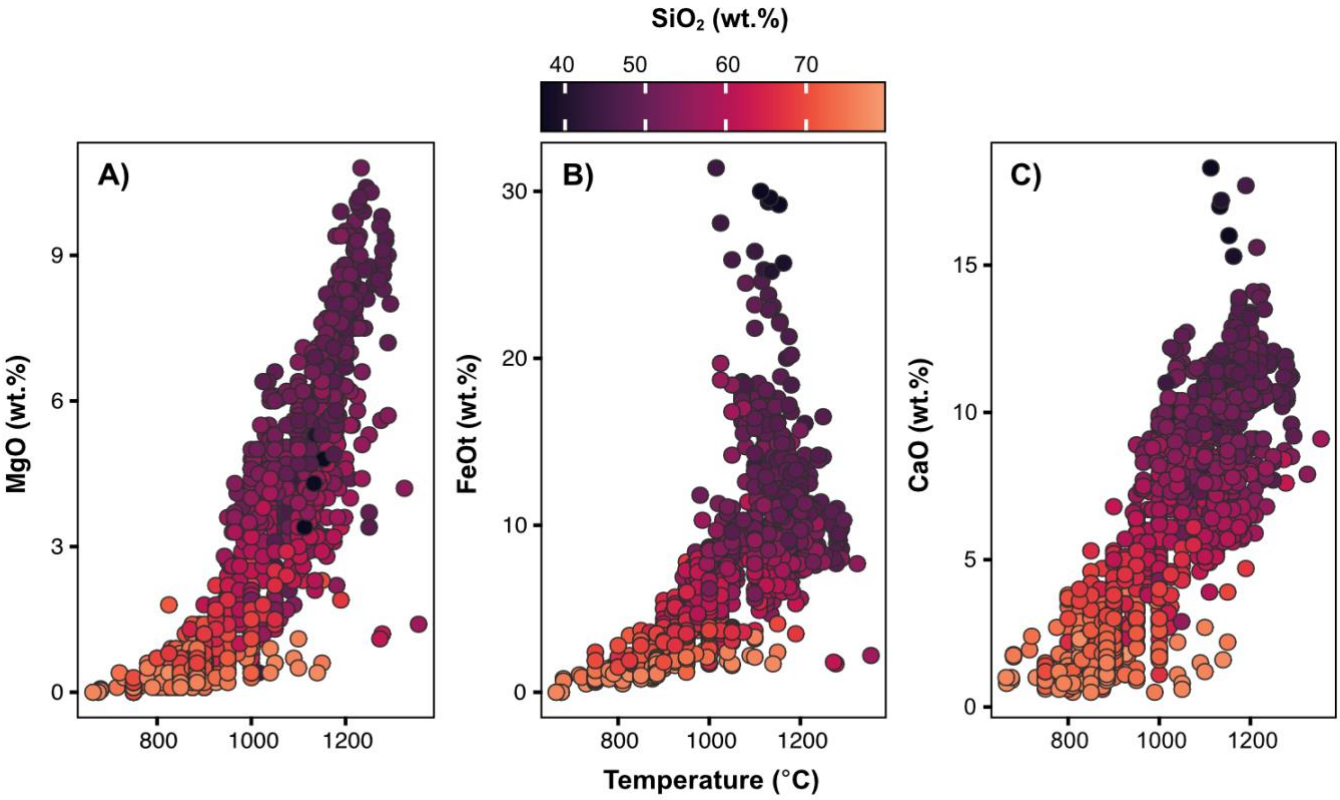
Appendix 1: Error propagation of temperature and water content estimates for hygrometry and barometry

The ML H_2O-independent thermometer and T-dependent hygrometer provides an uncertainty value (standard deviation; SD) from the T or H_2O prediction of each individual glass compositional analysis. For n=50, a uniform distribution within the SD on every temperature or water content estimate predicted by the H_2O-independent thermometer and T-dependent hygrometer is sampled. For example, if the thermometer returns a value of 900 °C and a SD of ± 50 °C, 50 points are sampled between 850–950 °C according to a uniform distribution. All 50 temperature/water content estimates are then input into the T-dependent hygrometer or H_2O-dependent barometer for each glass analysis. The maximum absolute difference to the mean value is the maximum uncertainty associated with a given pre-eruptive water content/pressure estimate.

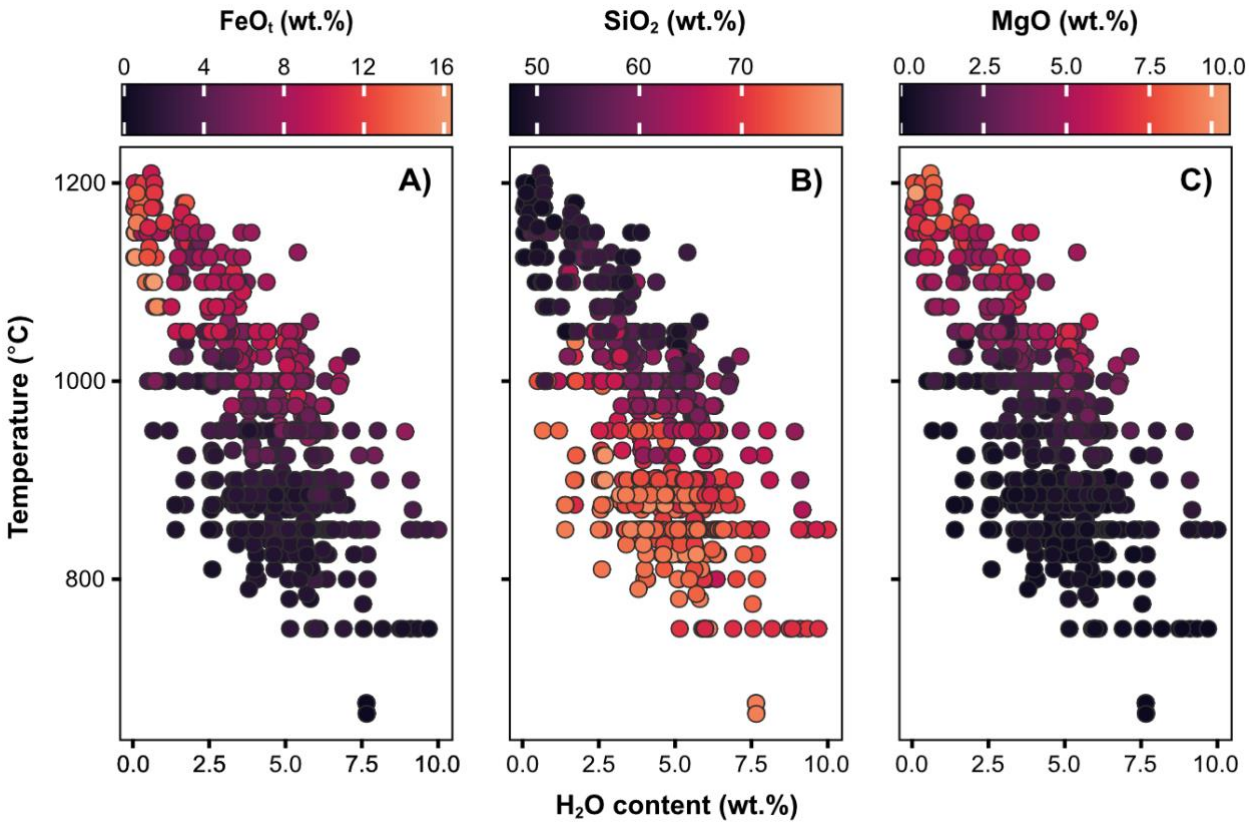
Supplementary Figures



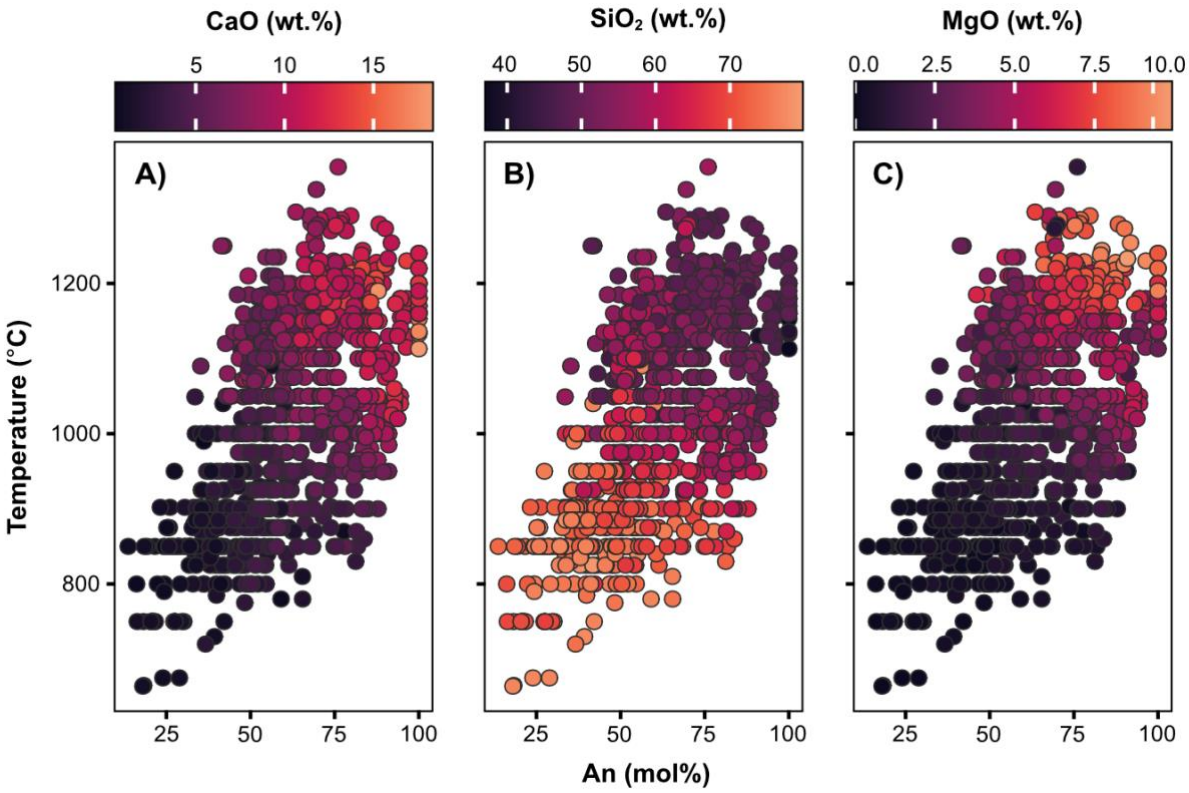
S.1: Plots of variable importance vs. input parameter for the H_2O-dependent thermometer (A), T-dependent hygrometer (B), and H_2O-dependent barometer (C), highlighting the most important variables used by the ExtraTrees algorithm to make predictions.



S.2: Plots illustrating the strong non-linearity between temperature and (A) MgO (wt.%), (B) FeOt (wt.%), and (C) CaO (wt.%) in the liquid. Colour coding reflects the SiO_2 (wt.%) of the liquid.



S.3: Temperature vs. H_2O (wt.%) of experimental glass compositions with colour coding showing the (A) FeO_t (wt.%), (B) SiO_2 (wt.%), and (C) MgO (wt.%) contents in the liquid.



S.4: Temperature of experimental glass compositions vs. An content (mol%) of experimental plagioclase with colour coding showing the (A) CaO (wt.%), (B) SiO_2 (wt.%), and (C) MgO (wt.%) contents in the liquid.