Supplementary Materials for…

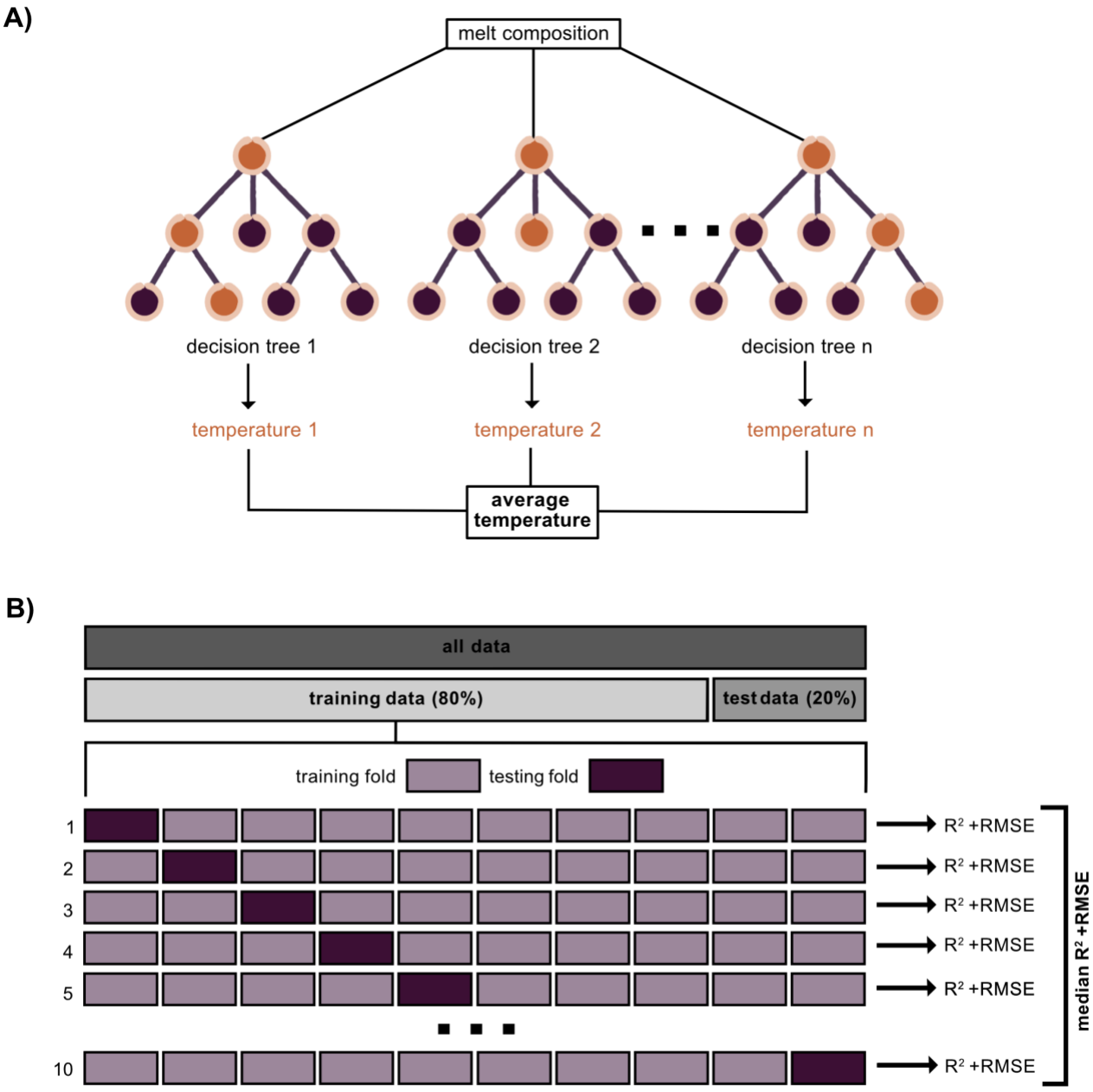
'Plagioclase-saturated melt hygrothermobarometry and plagioclase-melt equilibria using machine learning'

- **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.5** (p.3-7)

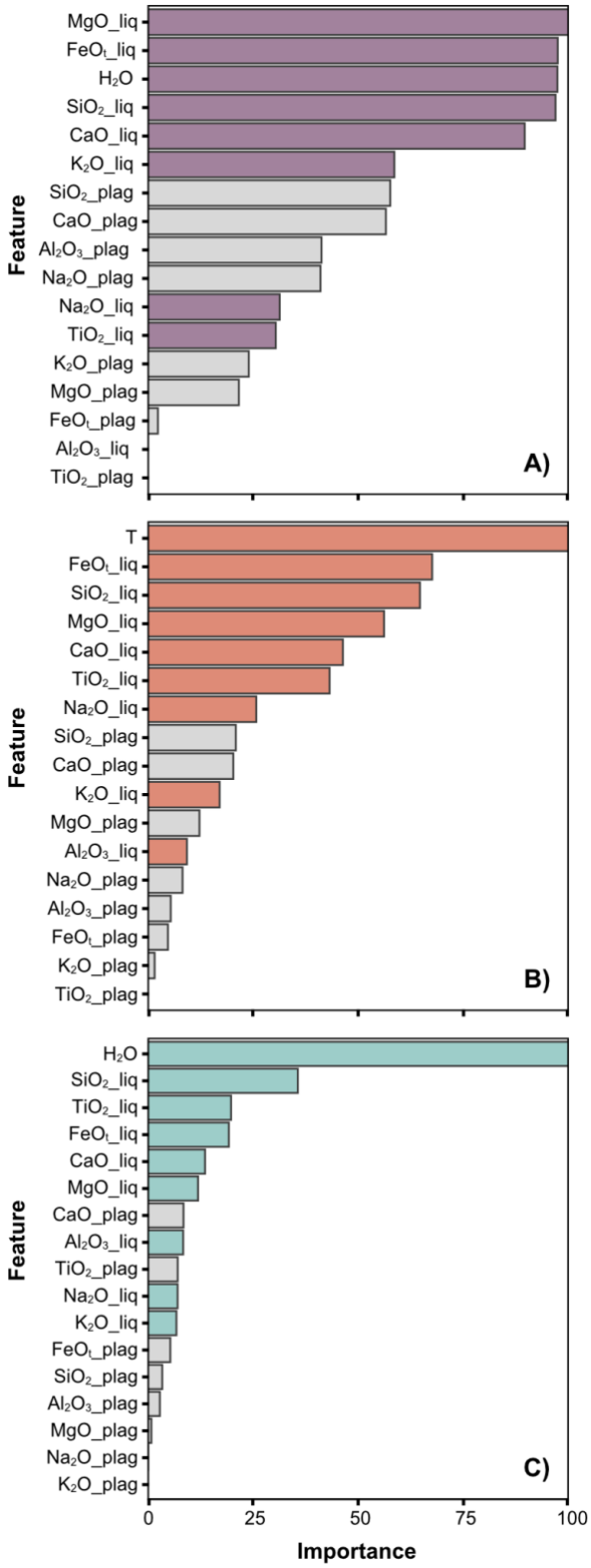
Appendix 1: Error propagation of temperature and water content estimates for hygrometry and barometry

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.

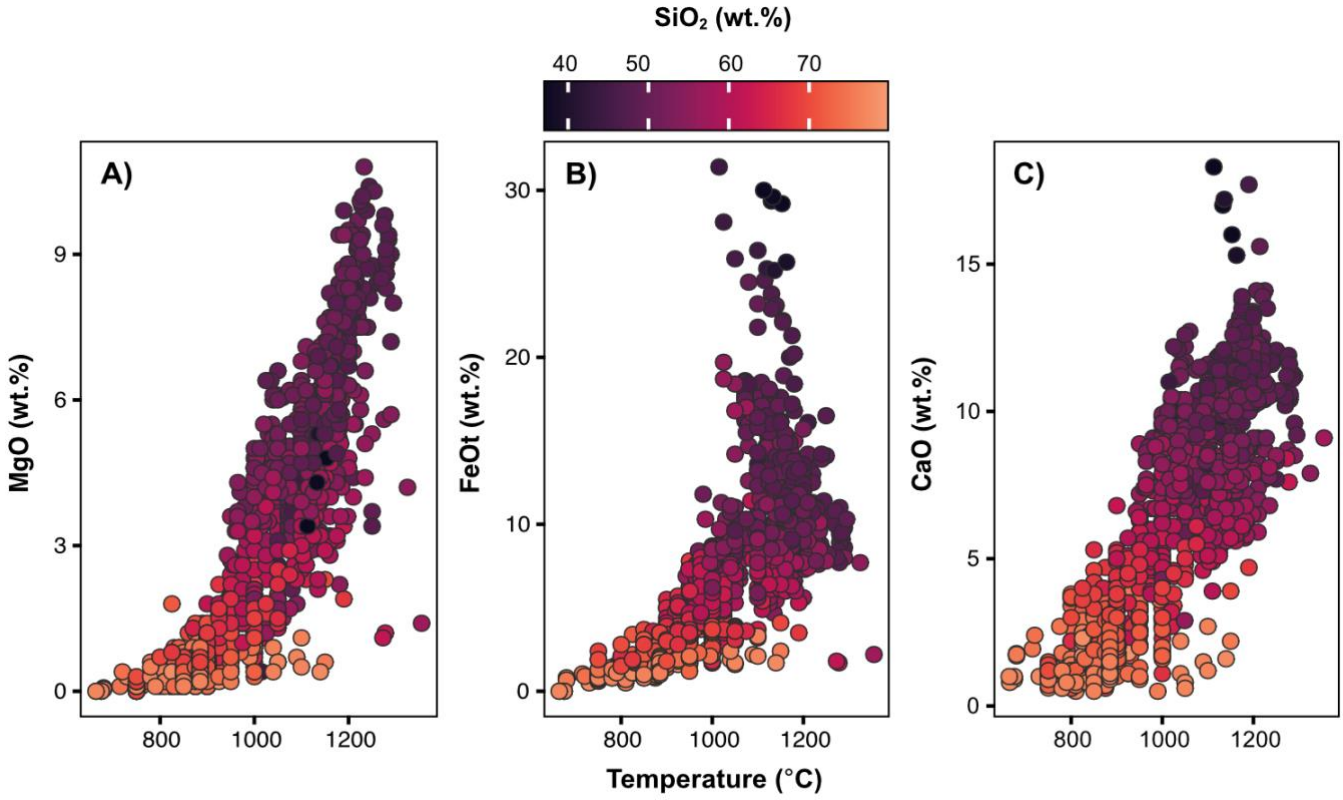
Supplementary Figures



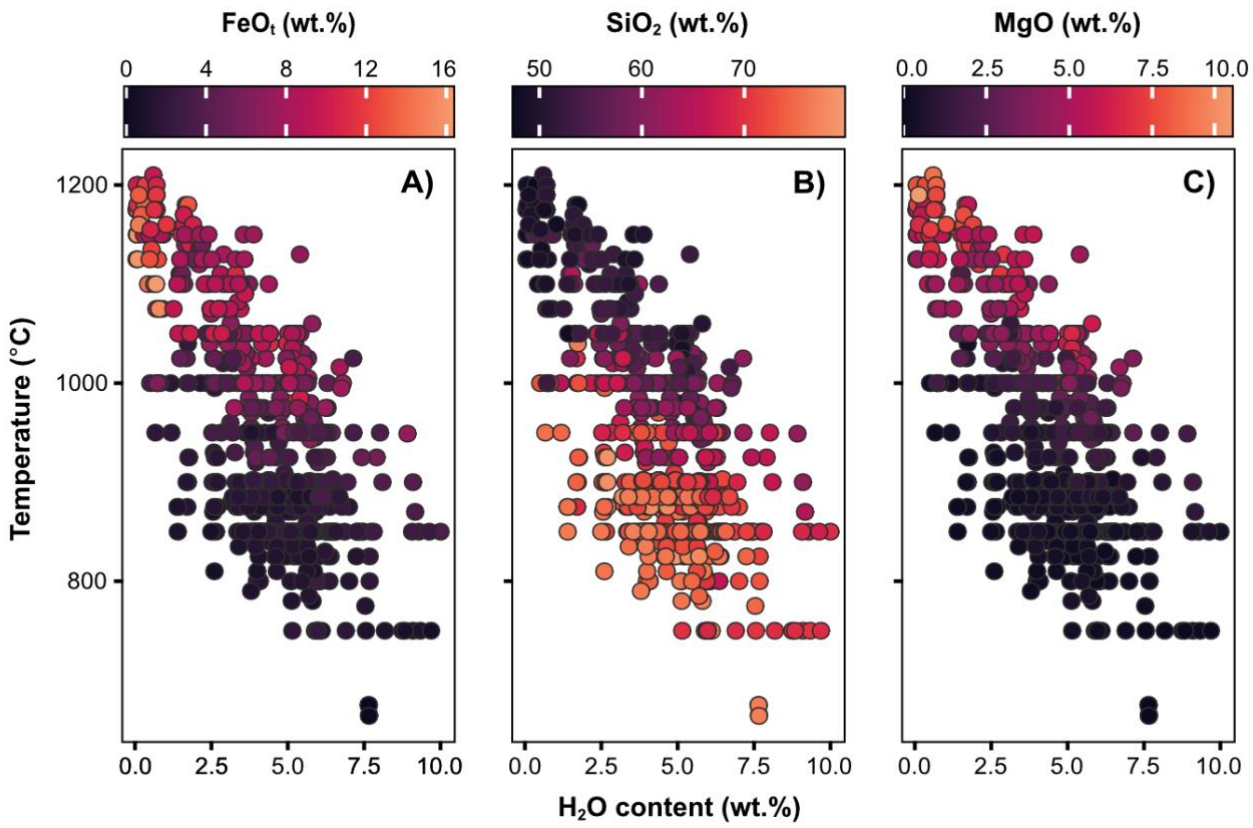
S.1: Summary diagrams of the random forest algorithm and the cross-validation process. A) Simplified diagram of a random forest thermometer displaying how a temperature prediction forms via averaging of multiple decision trees. B) Schematic of 10-fold cross-validation.



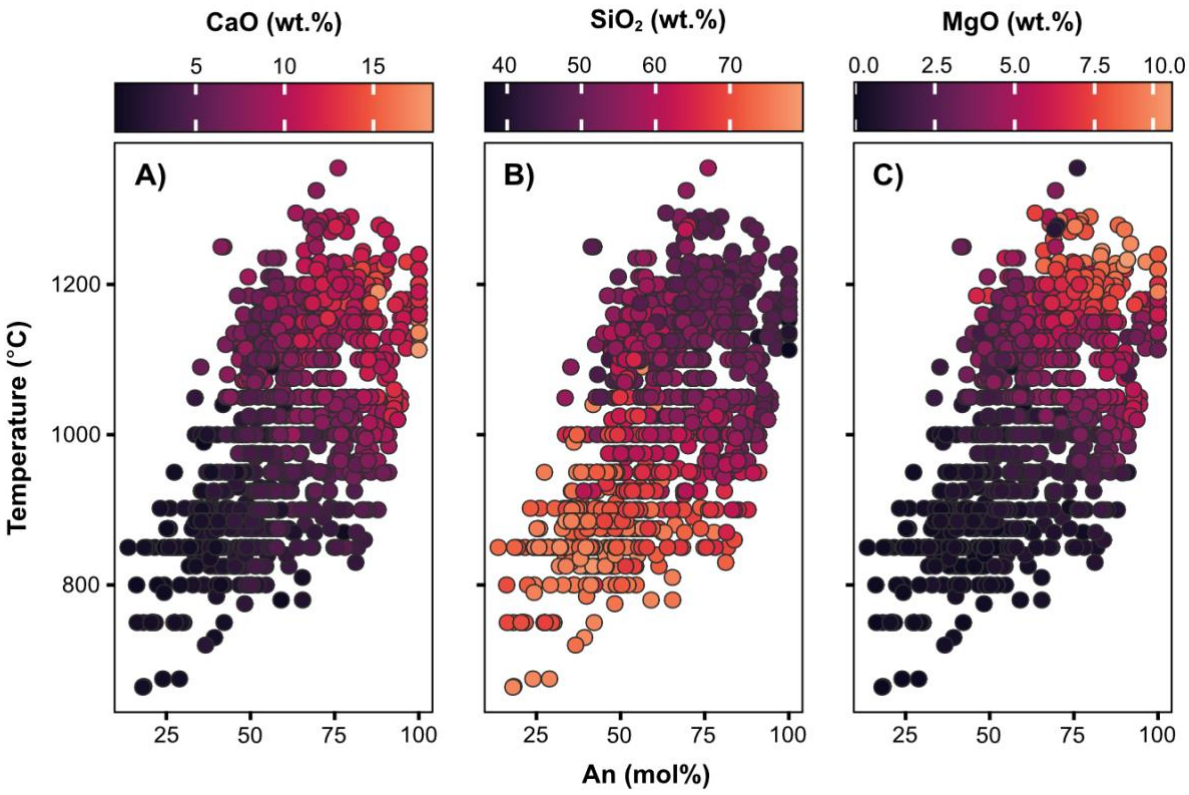
S.2: Plots of variable importance vs. input parameter for the H_2O-dependent thermometer (A), T-dependent hygrometer (B), and H_2O-dependent barometer (C), highlighting the most important variables used by the ExtraTrees algorithm to make predictions. Grey bars represent plagioclase compositional inputs and coloured bars represent liquid compositional inputs along with additional parameters such as T or H_2O.



S.3: 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.4: 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.5: 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.