Supplementary Text to:

"SilicH_2O: a graphical user interface for processing silicate glass Raman spectra and quantifying H_2O"

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CONTENTS

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1 Raman analytical methods

Instrument	Horiba Jobin LabRAM HR Evolution
Focal length	800 mm
Laser type	Nd:YAG
Laser wavelength	532.18 nm
Laser source power	100 mW
Grating	1800 grooves/mm
Confocal pinhole aperture	100–200 µm
Objective	100× magnification
Acquisition window	150–4000 cm^{-1}
Frame acquisition time	150 s
Accumulations	2
Total analysis time	~55 min

Table S1. Analytical settings for measuring silicate glasses with the KU Leuven Raman spectroscope.

All glasses were tested for sensitivity to the laser and where necessary laser power was reduced to 50% to prevent burning of the sample (Figure S1). Note that extra care has to be taken with long analyses like these, as samples may gradually heat up over time as they are exposed to the laser. Confocal pinholes of 100 µm were used for all validation and precision test analyses and 200 µm for calibration samples.

A calibration curve (Figure S2) was constructed from samples with H_2O contents between 0 and 6.4 wt.% (see Figure S3, Figure S4 and Supplementary Data for their major element compositions). Their H_2O contents were measured with a Cameca IMS 1270e7 Secondary Ion Mass Spectrometer (SIMS) at the Centre de Recherches Pétrographiques et Géochmiques (Nancy, France). Sample preparations and instrumental settings were the same as van Gerve et al., 2023, except that the samples were pressed in indium mounts.

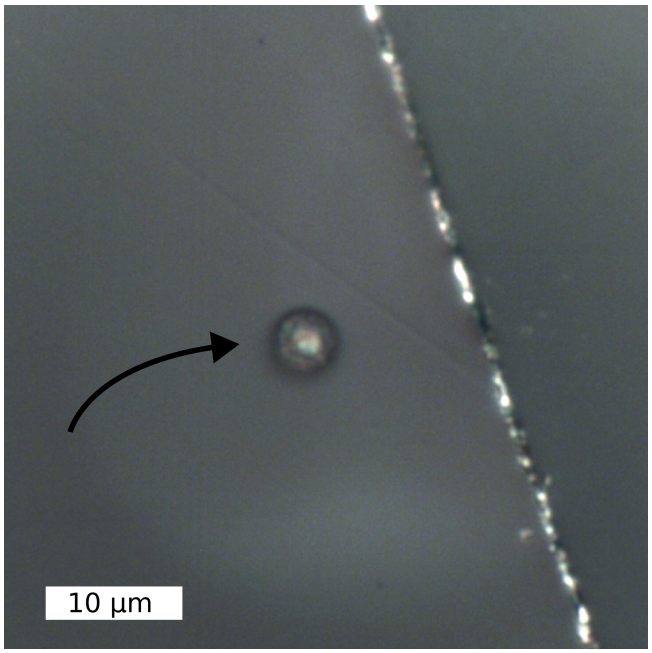

Figure S1. Glass burn damage from the laser

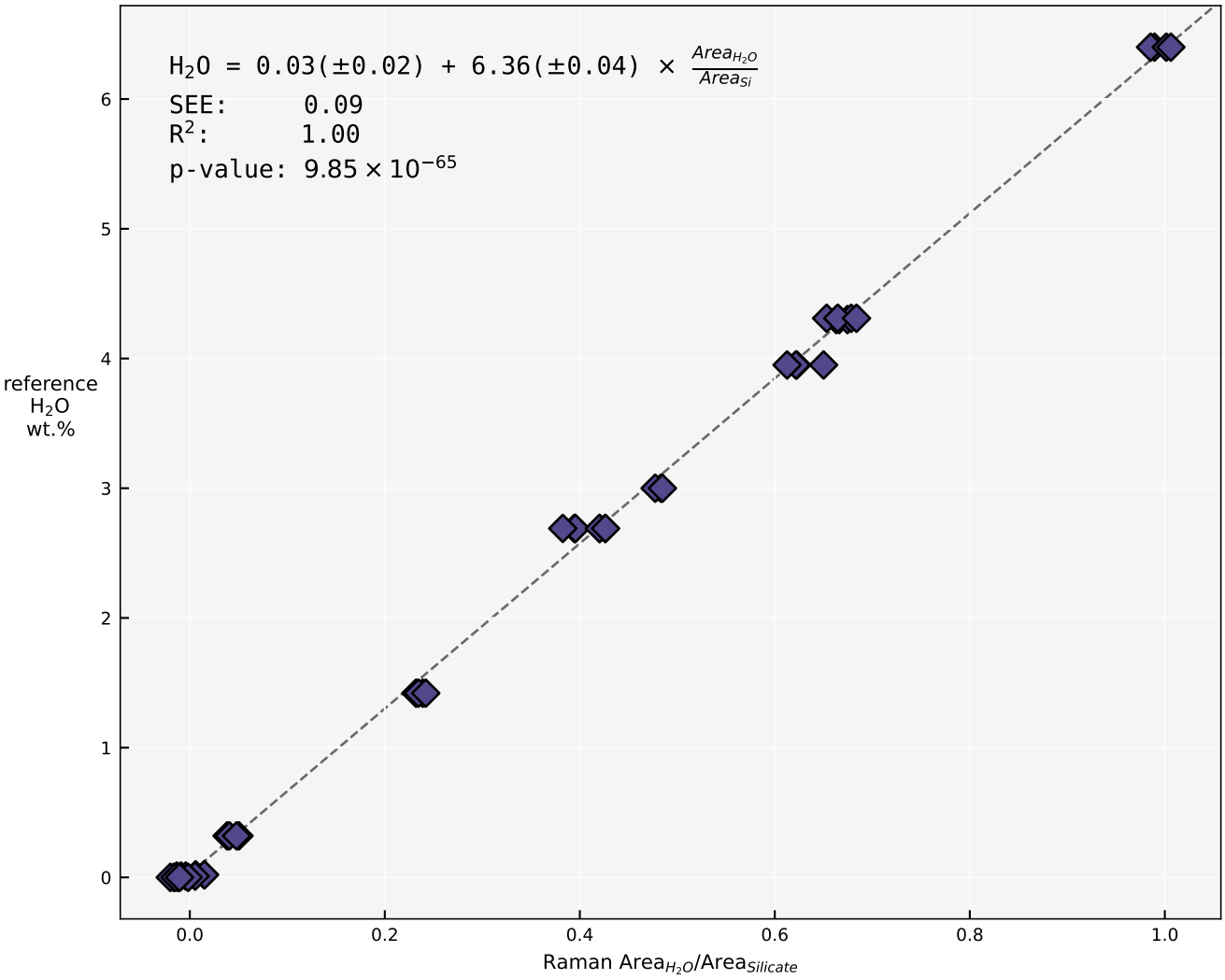

Figure S2. KU Leuven Raman H_2O calibration curve

2 Plots of validation and calibration samples

Sample lists and Raman results of validation and calibration samples are provided as excel files in the Supplementary data.

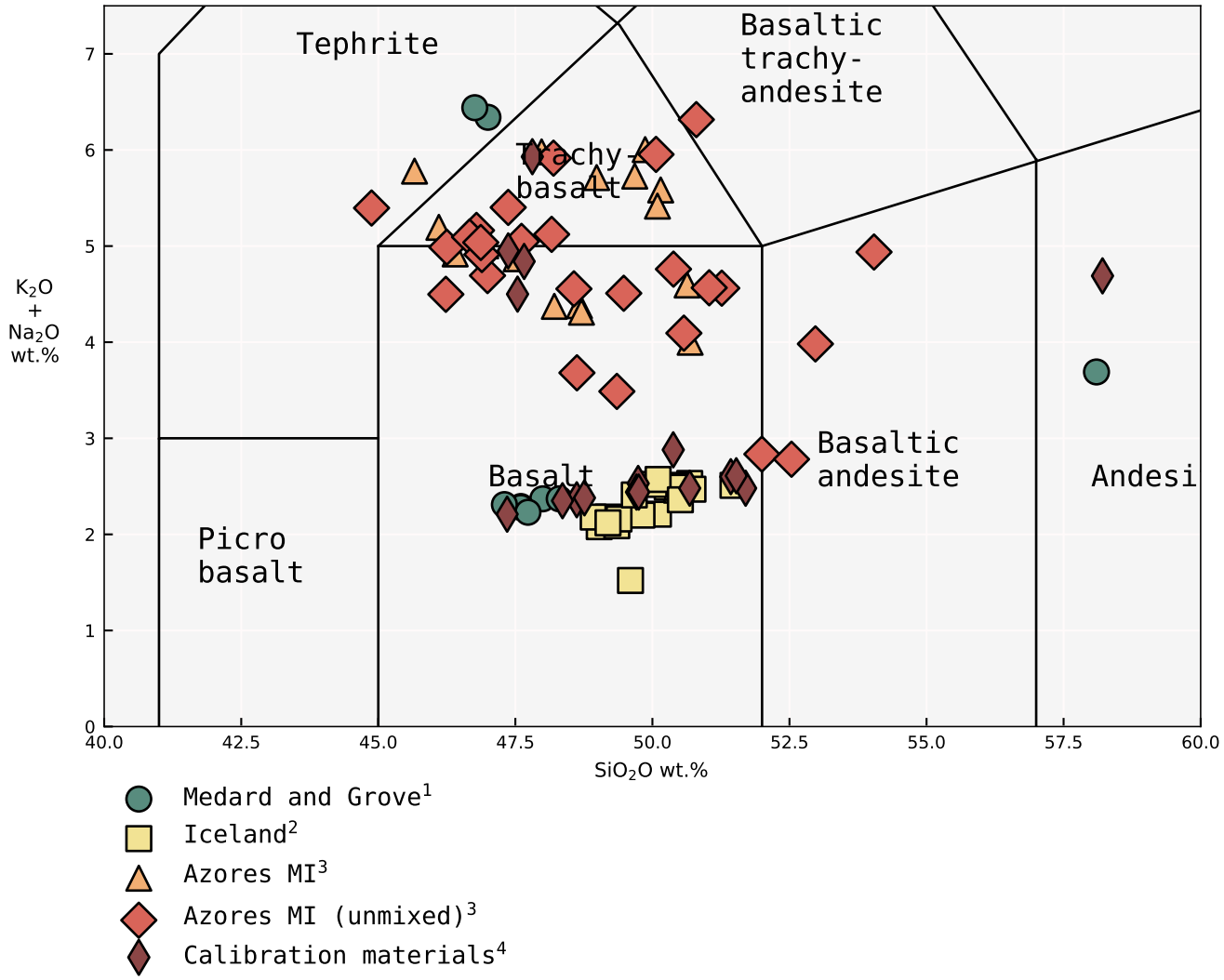

Figure S3. Total alkali contents as a function of silica content for calibration and validation samples. [1]Médard and Grove, 2008, [2]Neave et al., 2019, [3]van Gerve et al., 2023, under review, [4]Duggen et al., 2007; Jochum et al., 2006; Shishkina et al., 2010

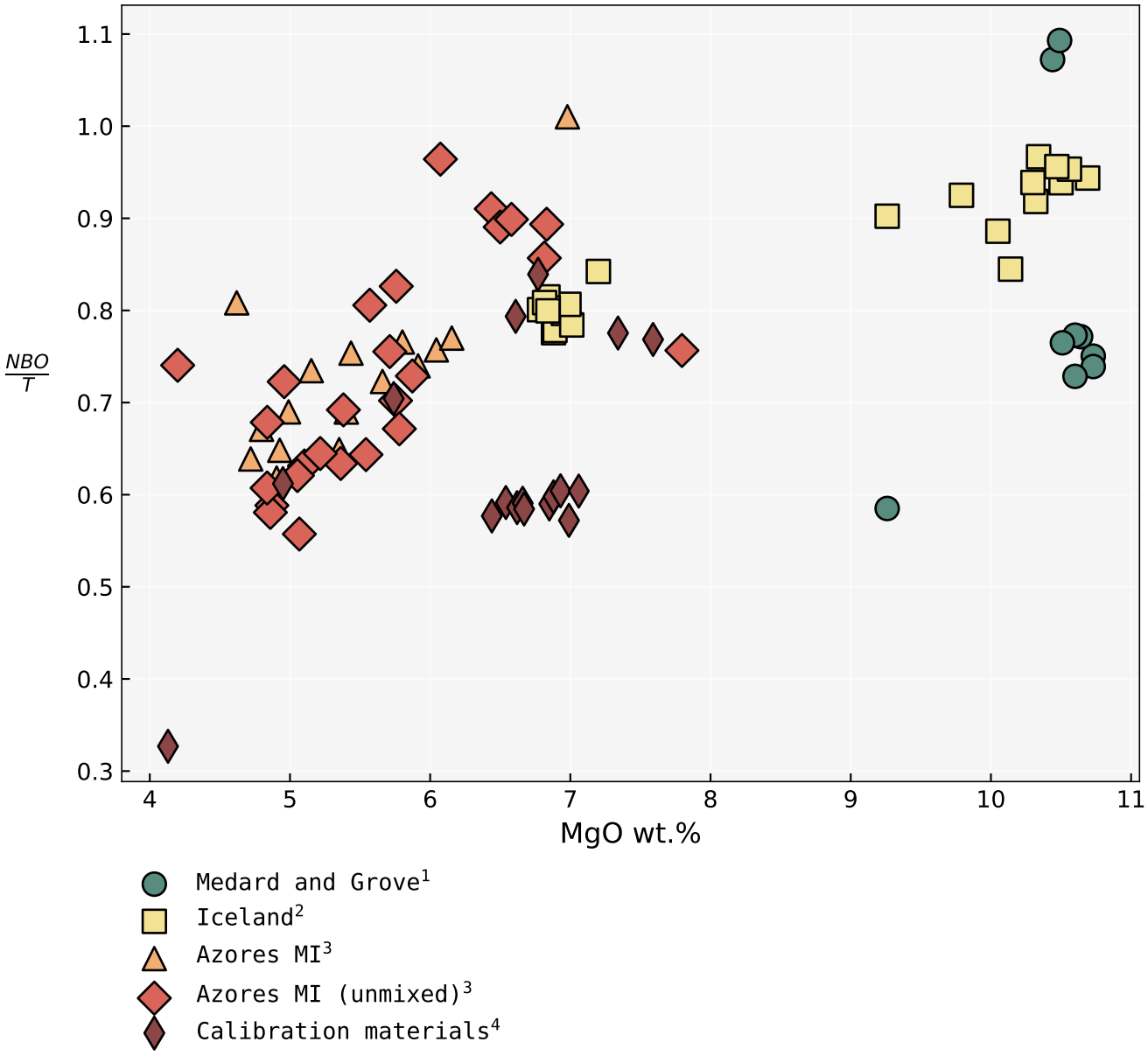

Figure S4. NBO/T (calculated following Mysen and Virgo, 1980) as a function of MgO content for calibration and validation samples. [1]Médard and Grove, 2008, [2]Neave et al., 2019, [3]van Gerve et al., 2023, under review, [4]Duggen et al., 2007; Jochum et al., 2006; Shishkina et al., 2010

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