

Figure 1. N₂O data corrections flowchart. Instrument checks, pre-scrambling data corrections, the scrambling calibration, and isotopomer calculations are laid out; numbers in yellow circles correspond to step numbers referred to in the text. Steps 1-4 are performed with raw Isodat output, steps 5-8 are accomplished in the data corrections spreadsheet template, step 9 is a simple calculation, and steps 10-14 are accomplished with the pyisotopomer code.

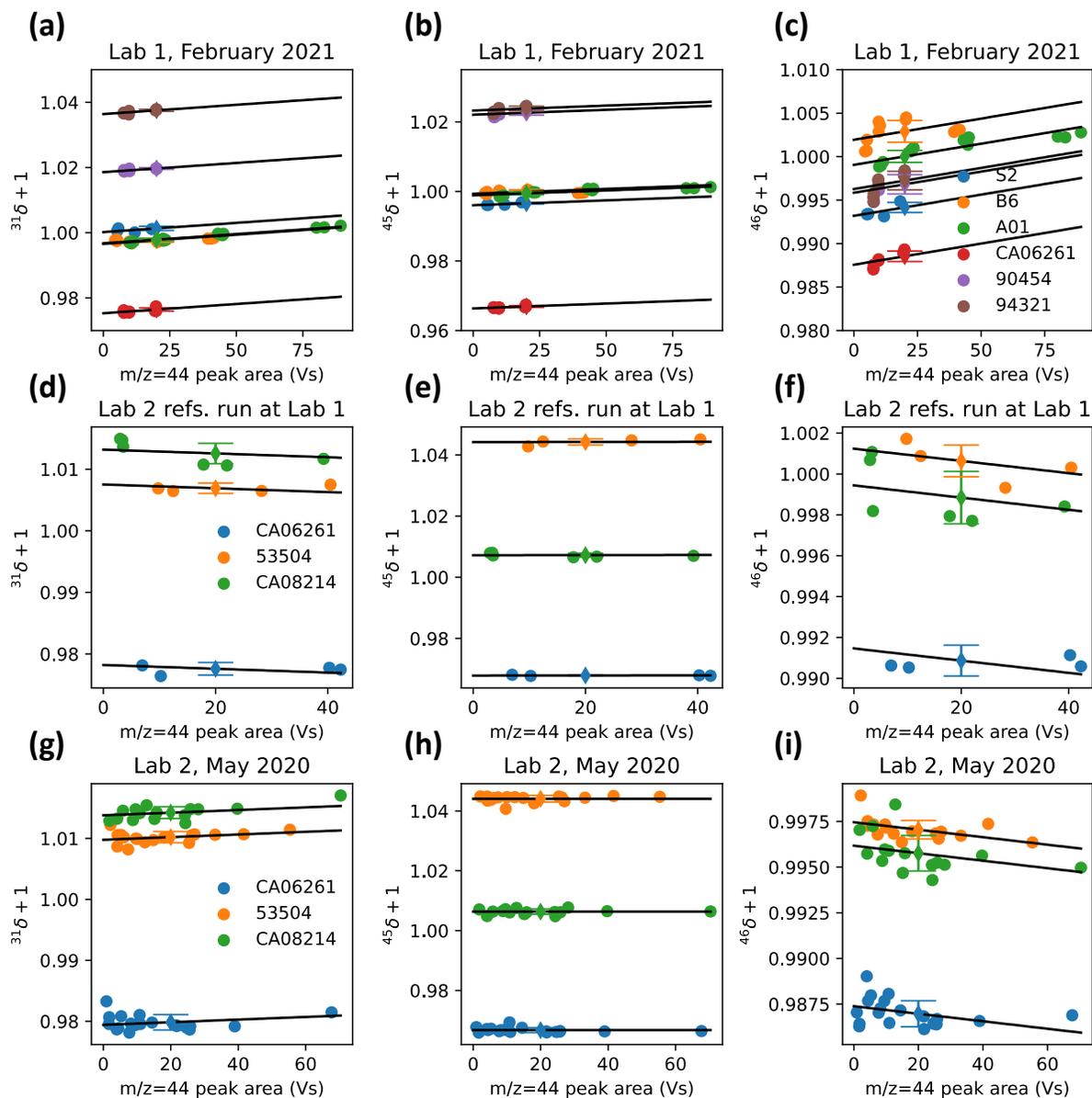


Figure 2. Linearity relations for reference materials used to normalize measured isotope ratios to a peak area of 20 Vs, using the dummy variable method⁶⁷. $^{31}\delta+1$ (a,d,g), $^{45}\delta+1$ (b,e,h), and $^{46}\delta+1$ (c, f, i) are plotted against m/z 44 peak area. Linearity relations are shown for reference materials prepared and run in Lab 1 (a-c), reference materials prepared in Lab 2 but run in Lab 1 (d-f), and reference materials run in Lab 2 (g-i). A common slope (black line) calculated from the dummy variable method for each molecular ion ratio is overlain on each data series (colored circles). The estimated isotope ratio corresponding to a peak area of 20 Vs is also shown for each series (colored diamonds, error bars correspond to the standard error of the predicted y-value).

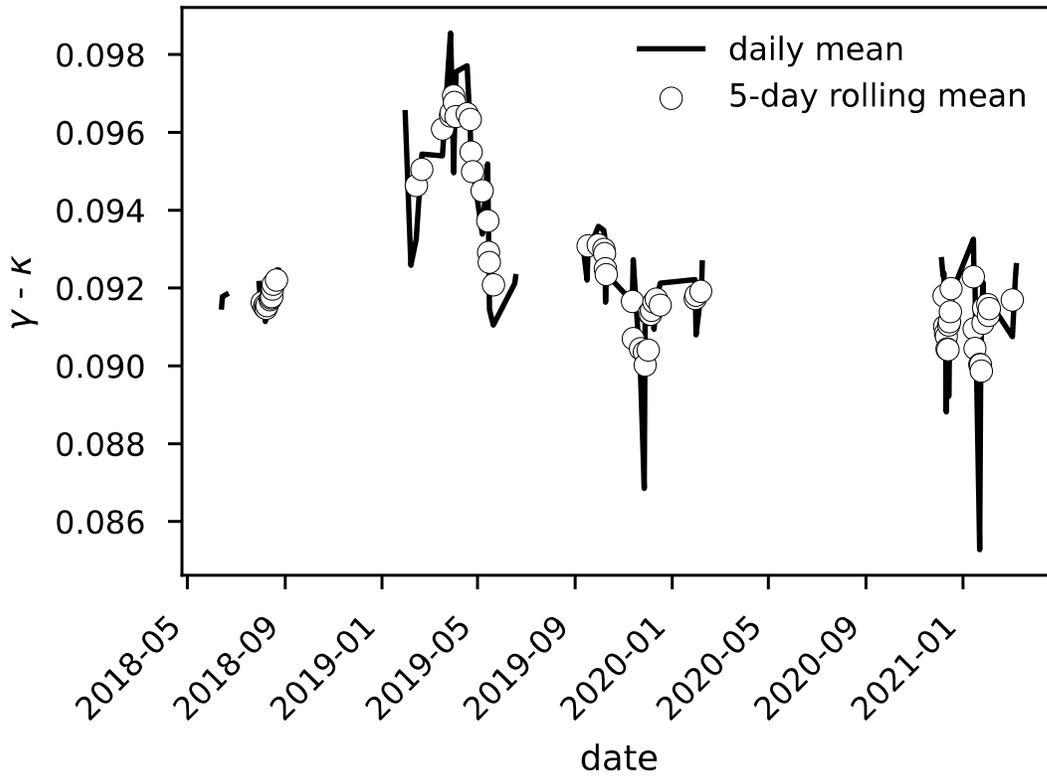


Figure 3. $\gamma - \kappa$ for the Lab 1 IRMS from June 2018 to March 2021. Daily mean $\gamma - \kappa$ (black line) values are plotted with a 5-day rolling average (dots).

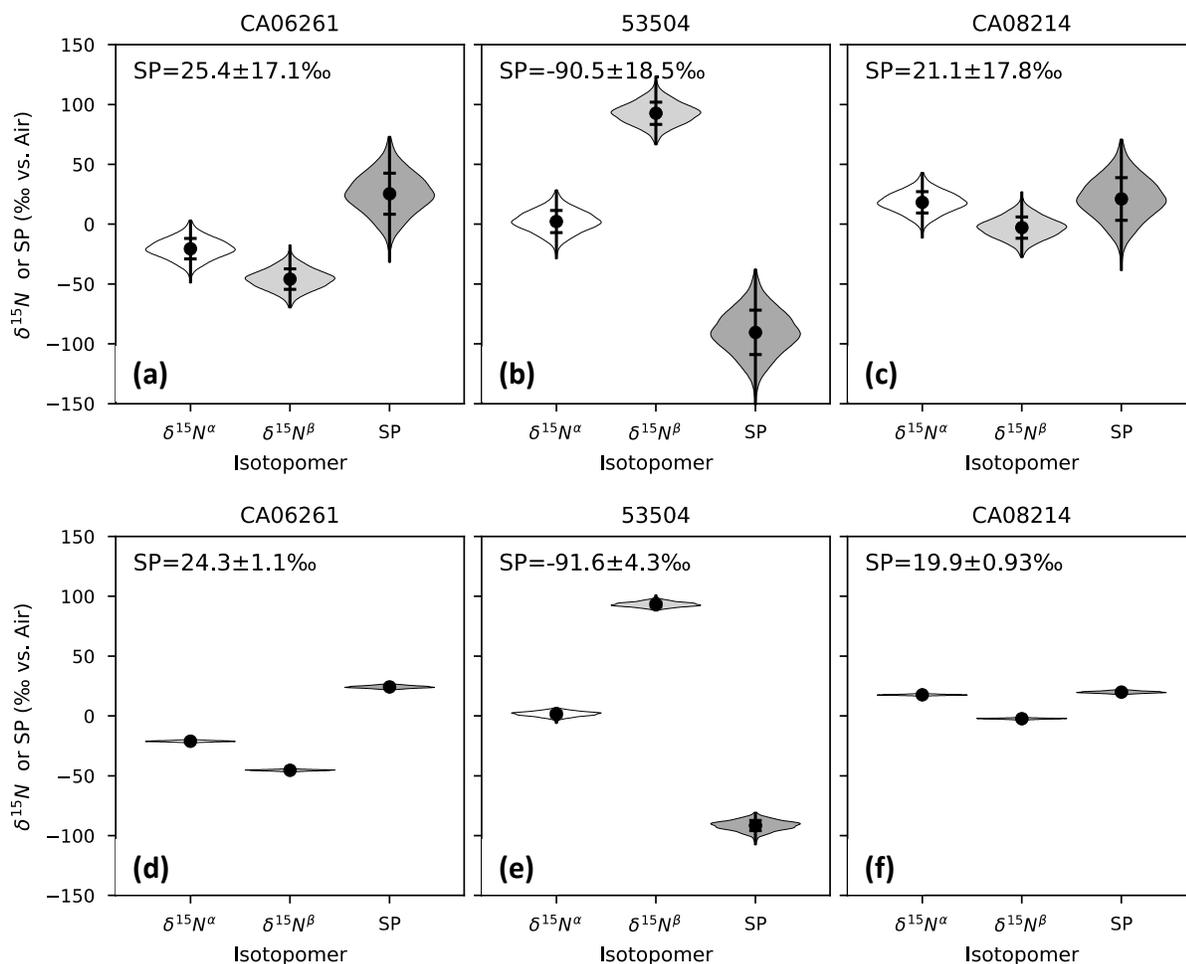


Figure 4. a-c) Isotopocule values and error associated with a 10 % relative uncertainty in $\gamma - \kappa$, based on Monte Carlo simulation results, for reference materials CA062621 (a), 53504 (b), and CA08214 (c). γ and κ were modeled as random numbers centered around $\gamma = 0.174$ and $\kappa = 0.083$, with the uncertainty in $\gamma - \kappa$ equal to 10 % of the mean $\gamma - \kappa$ (0.091). d-f) Isotopocule values and error associated with a 10% relative uncertainty in the absolute values of $\gamma - \kappa$, holding the difference $\gamma - \kappa$ constant, for reference materials CA062621 (d), 53504 (e), and CA08214 (f). γ and κ were modeled in tandem as random numbers centered around $\gamma = 0.174$ and $\kappa = 0.083$, with uncertainties equal to 10% of the mean γ , and $\gamma - \kappa$ was held constant at 0.091. Violin plots are based on a kernel density estimate of the distribution and the values plotted and reported on each figure show the mean value $\pm 1\sigma$.