

Supplementary Information to ‘Double dating in the Middle Pleistocene: assessing the consistency and performance of the carbonate U–Th and U–Pb dating methods’

Timothy J. Pollard, Jon D. Woodhead, Russell N. Drysdale, R. Lawrence Edwards, Xianglei Li, Ashlea N. Wainwright, Mathieu Pythoud, Hai Cheng, John C. Hellstrom, Ilaria Isola, Eleonora Regattieri, Giovanni Zanchetta, and Dylan S. Parmenter

S1 Collector configuration for U–Th analyses

Table S1. Collector configuration for U–Th measurements. U and Th measurements were performed separately in static mode. An axial secondary electron multiplier (SEM) at mass position 237 was used to monitor and correct for tailing of the $^{238}\text{U}^+$ beam onto the other detectors during U measurement.

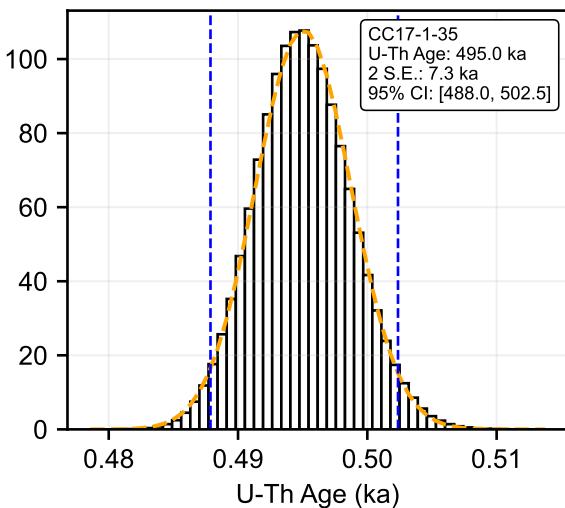
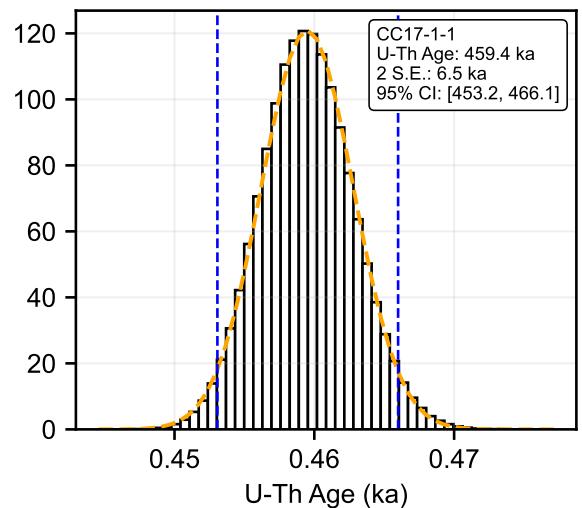
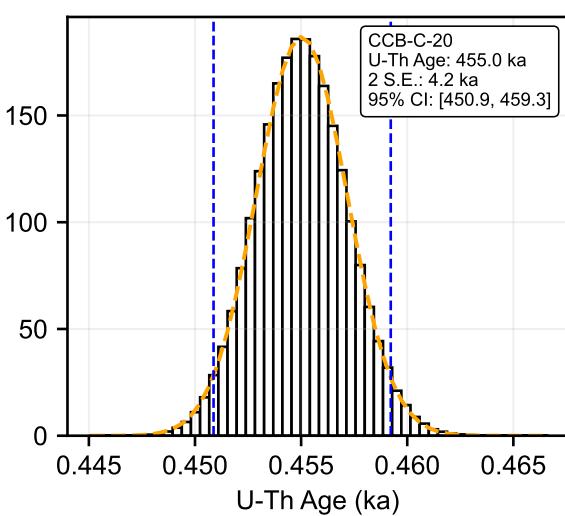
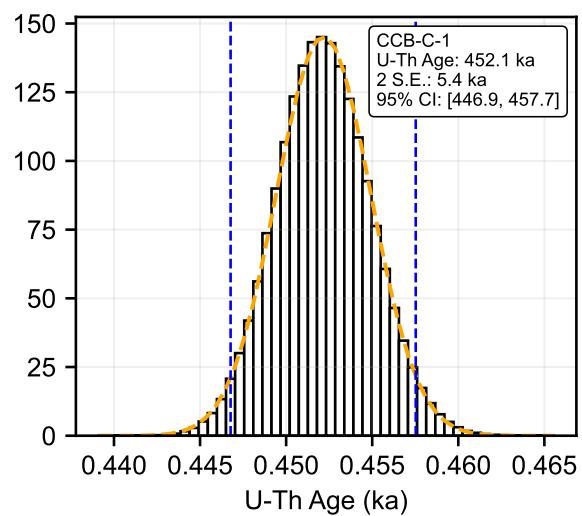
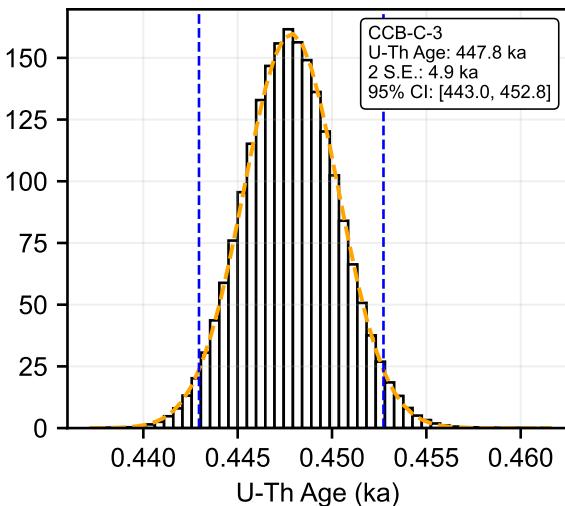
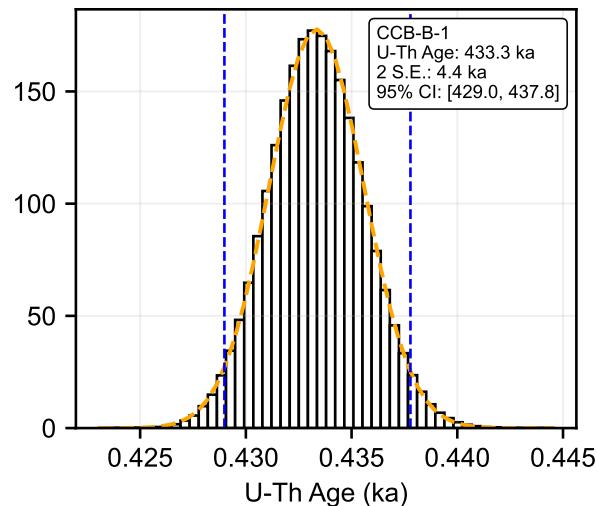
| Detector | L4 | L3 | L2 | L1 | Ax | H1 |
|---------------------------------|-------------------|-------------------|------------------|-------------------|-------|------------------|
| Position | −4 | −3 | −2 | −1 | 0 | +1 |
| Amplifier resistor (Ω) | 10^{11} | 10^{13} | 10^{11} | 10^{11} | (SEM) | 10^{10} |
| U isotope | ^{233}U | ^{234}U | ^{235}U | ^{236}U | 237 | ^{238}U |
| Th isotope | ^{229}Th | ^{230}Th | | ^{232}Th | | |

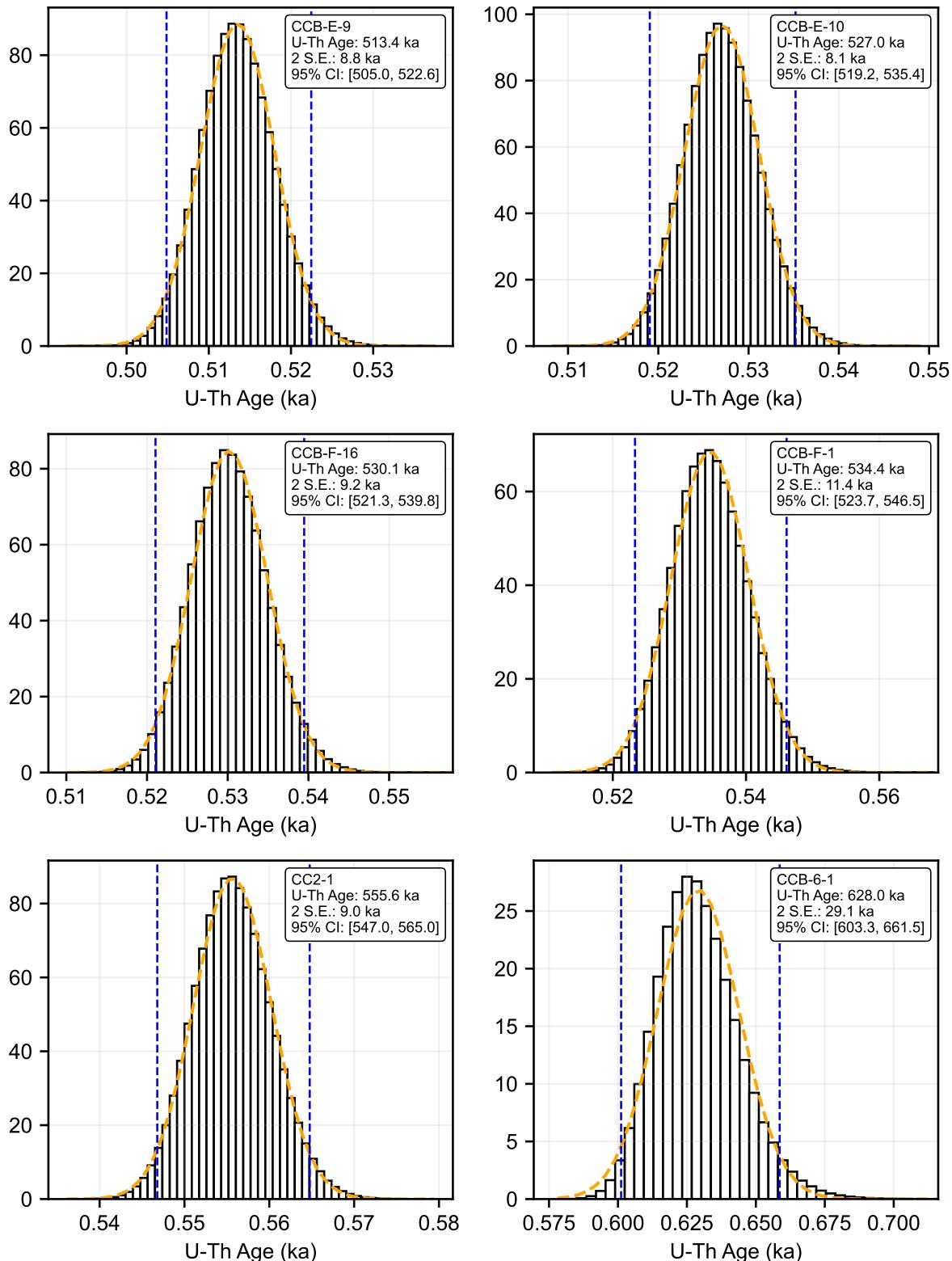
S2 Monte Carlo age simulation

Monte Carlo simulation (e.g. Hellstrom, 1998; Ludwig, 2003) was used to calculate U–Th and U–Pb age uncertainties, as well as estimate uncertainty on the age differences. For each trial:

- [$^{234}\text{U}/^{238}\text{U}$] and [$^{230}\text{Th}/^{238}\text{U}$] values were randomised within their analytical uncertainties according to univariate Gaussian distributions.
- U–Pb isochron regression parameters were randomised within uncertainties according to a multivariate Gaussian distribution accounting for uncertainty correlation between the slope and y -intercept.
- U–Th and U–Pb ages were calculated numerically using the equations outlined in Broecker (1963) and Pollard et al. (2023) (after Ludwig, 1977), and then checked for convergence.
- The difference between the U–Th and U–Pb ages was calculated.

This procedure was then repeated 10^6 times for each sample to build up an estimate of the probability density function for U–Th and U–Pb ages, and the age difference. Uncertainties are reported as 95% confidence intervals, estimated from the 2.5 and 97.5 percentiles of simulated ages (i.e. using the probabilistically symmetrical approach described by JCGM (2008))





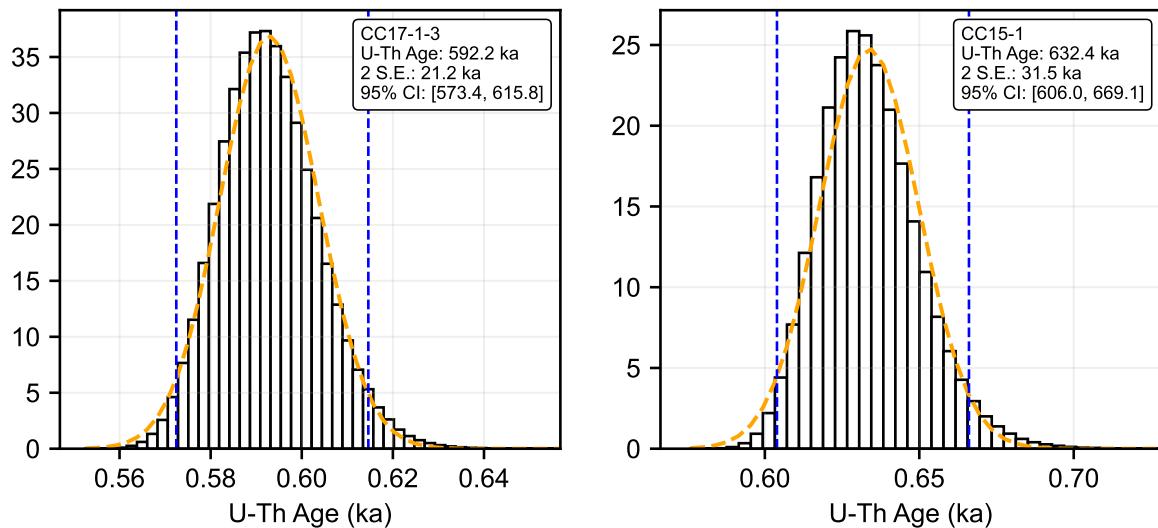
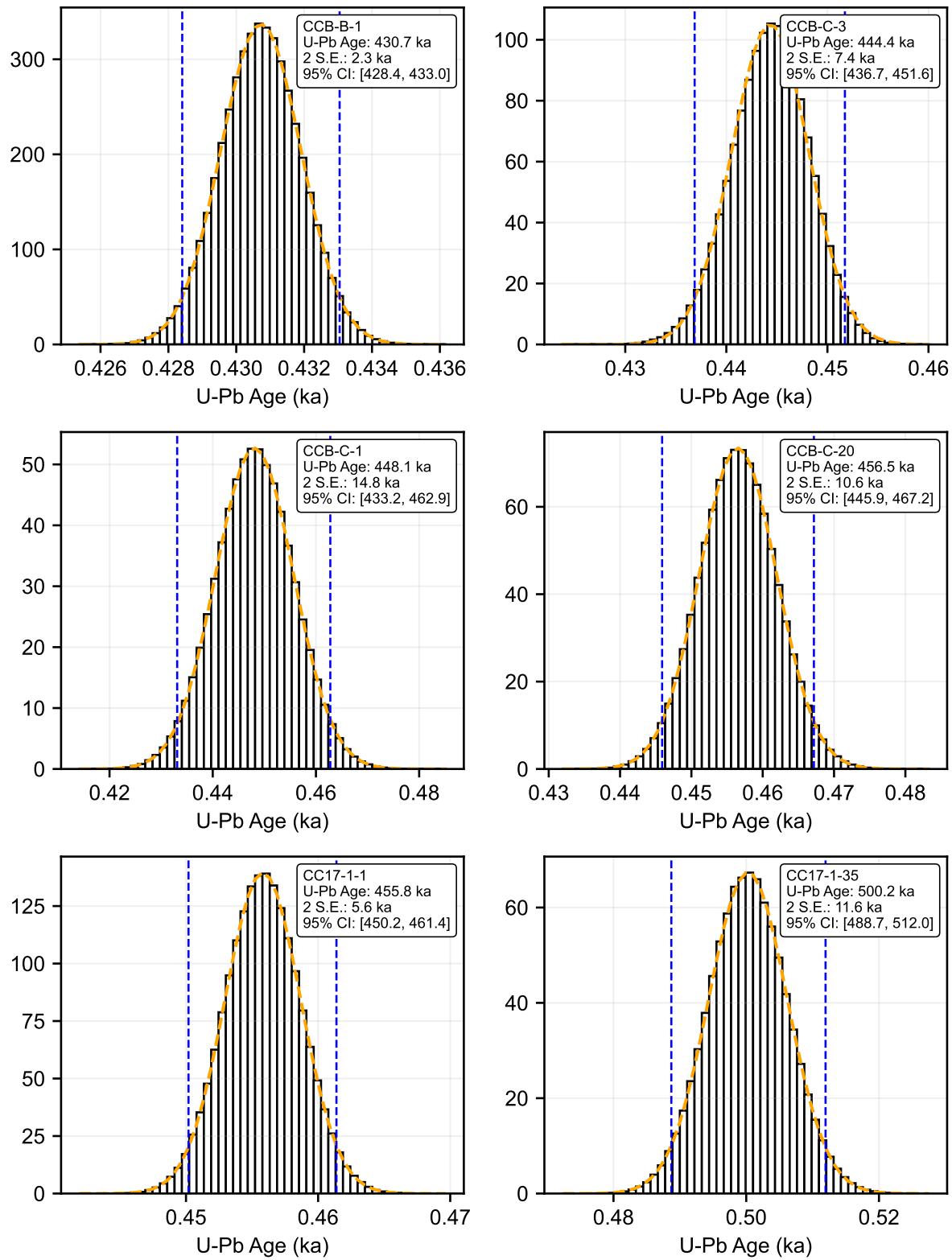
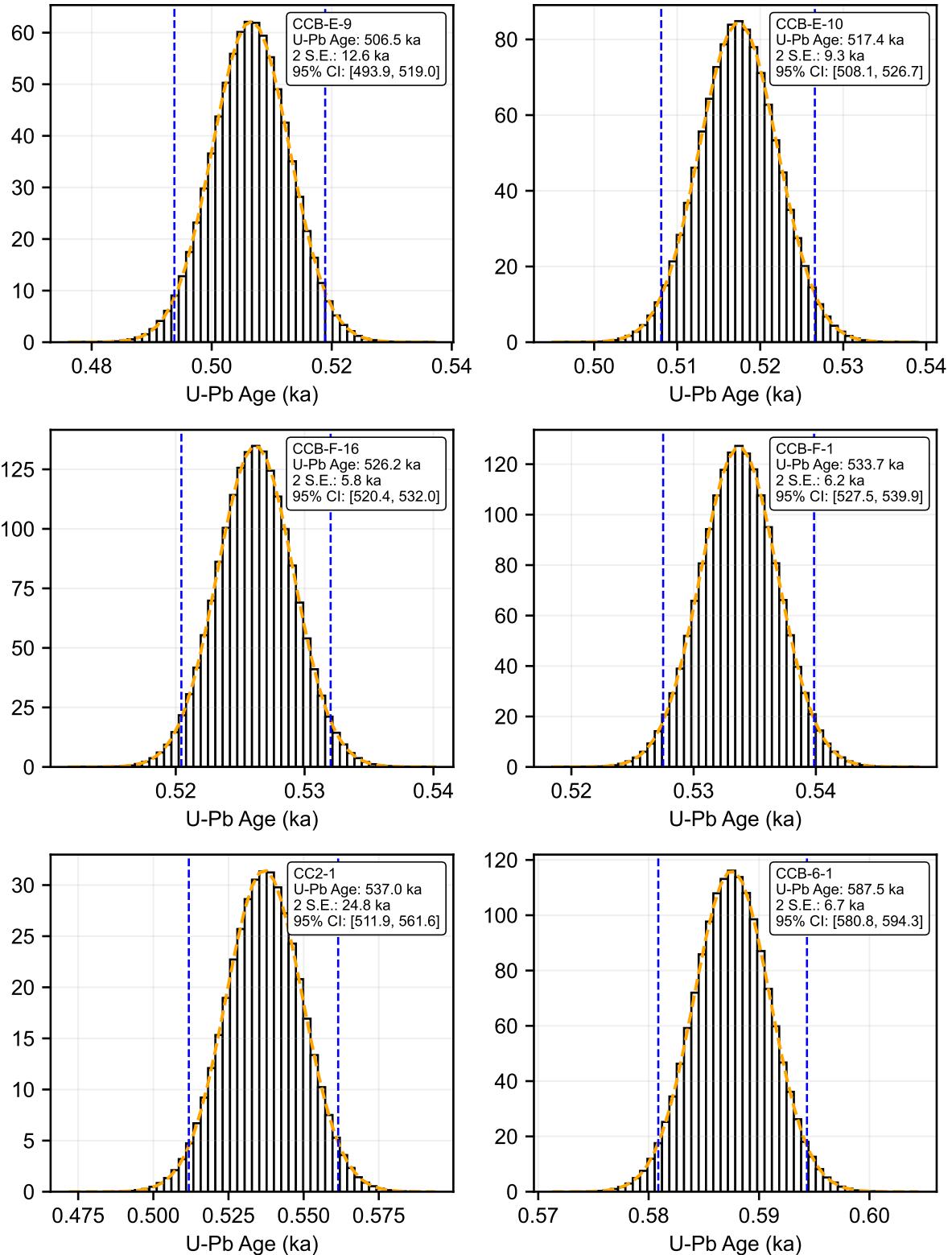


Figure S1. Histograms showing the results of U–Th Monte Carlo age simulations. The orange curve shows a Gaussian fit to the simulated ages, and the blue vertical lines show estimated 95% confidence limits.





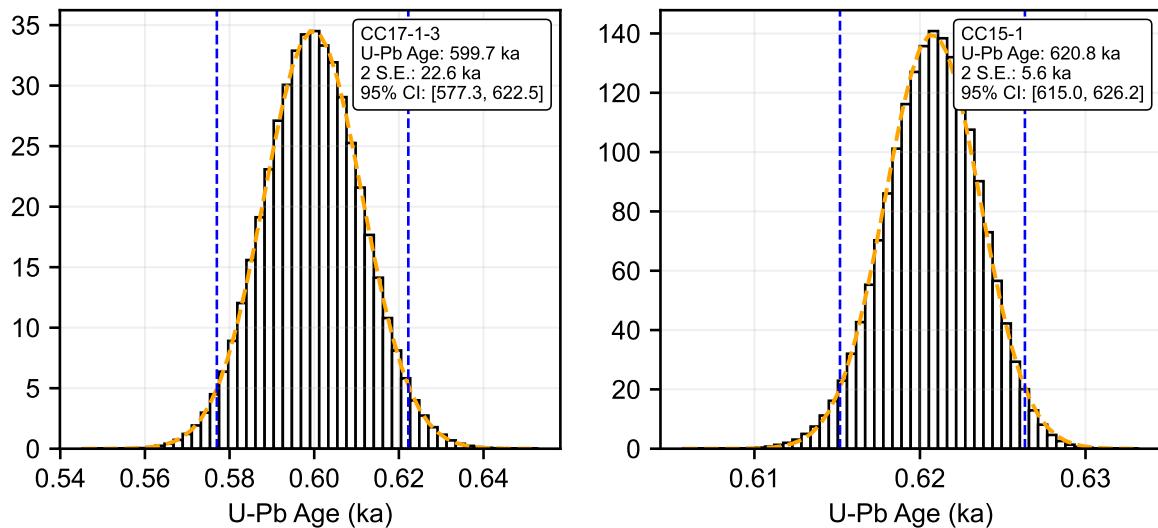
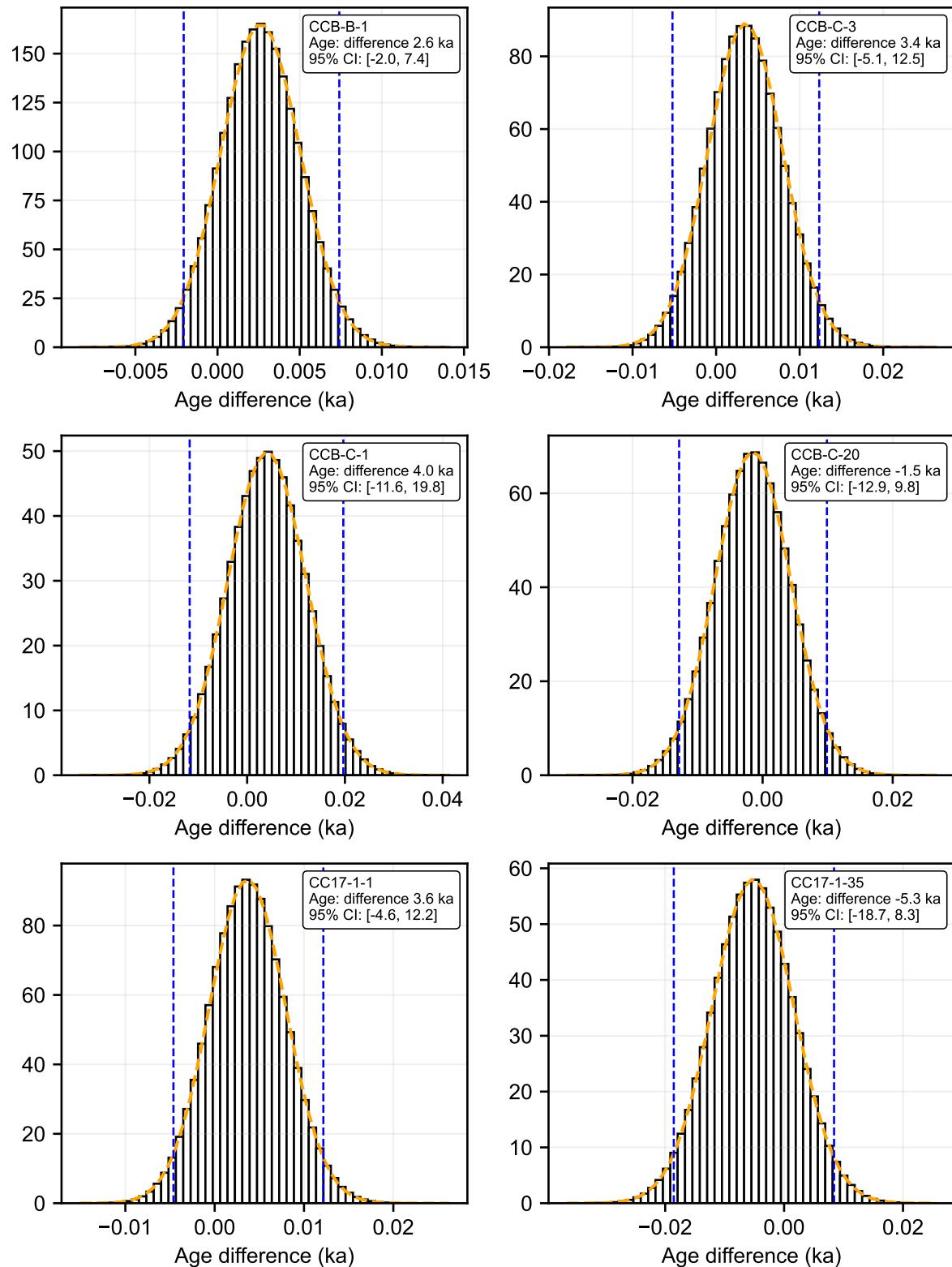
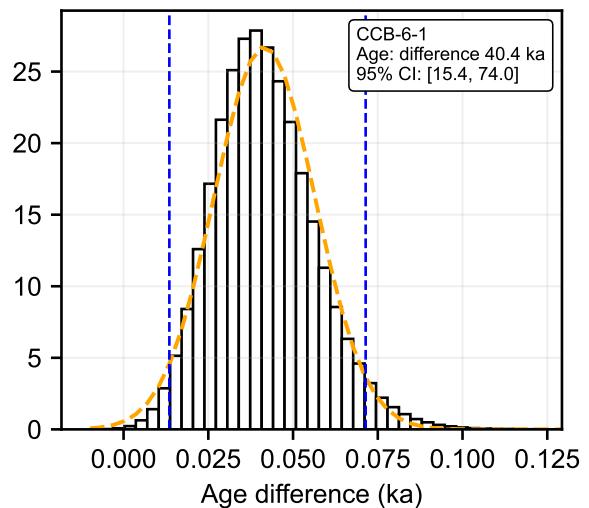
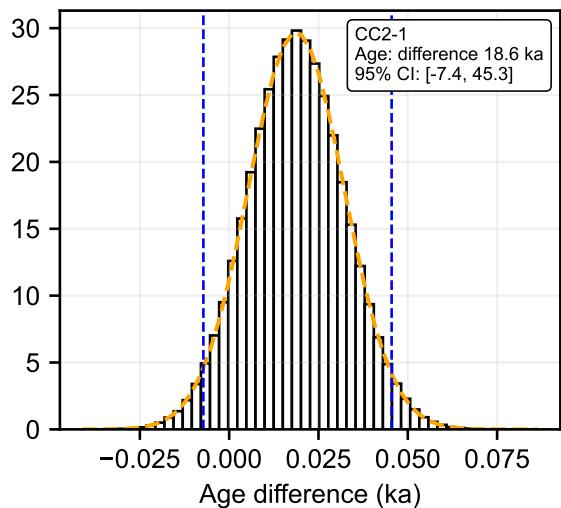
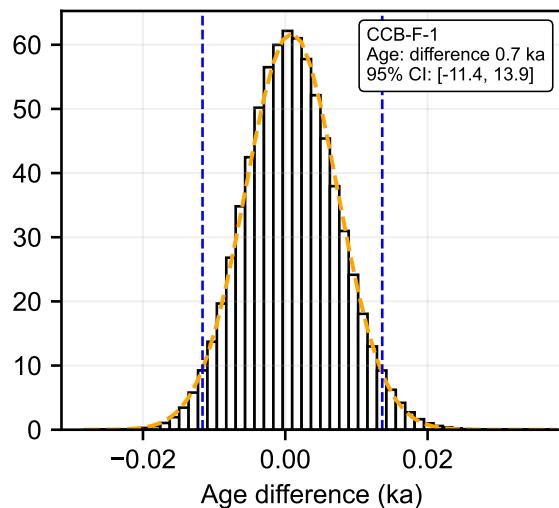
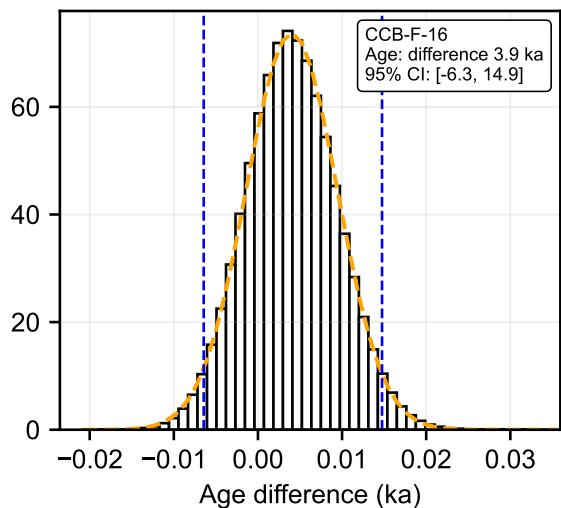
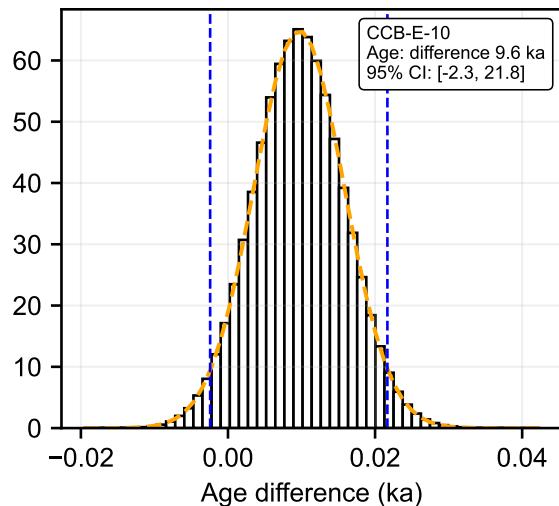
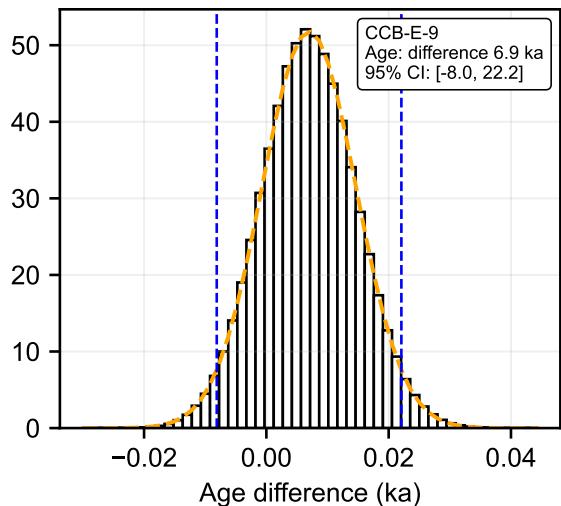


Figure S2. Histograms showing the results of U–Pb Monte Carlo age simulations. The orange curve shows a Gaussian fit to the simulated ages, and the blue vertical lines show estimated 95% confidence limits.





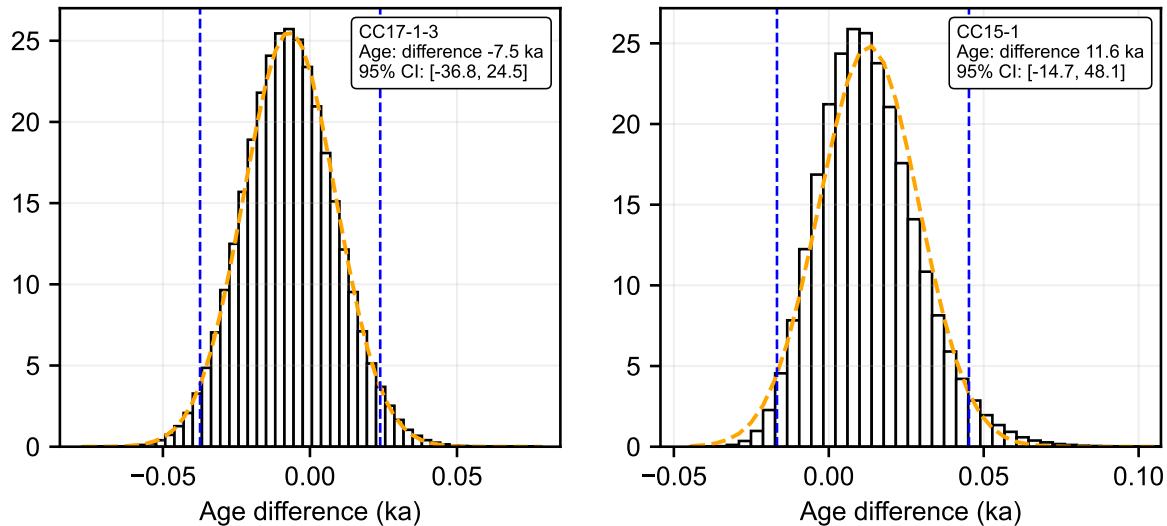


Figure S3. Histograms showing the results of Monte Carlo age difference simulations (i.e. U - Th age – U - Pb age). The orange curve shows a Gaussian fit to the simulated ages, and the blue vertical lines show estimated 95% confidence limits.

S3 Spread of data along the U–Pb isochron

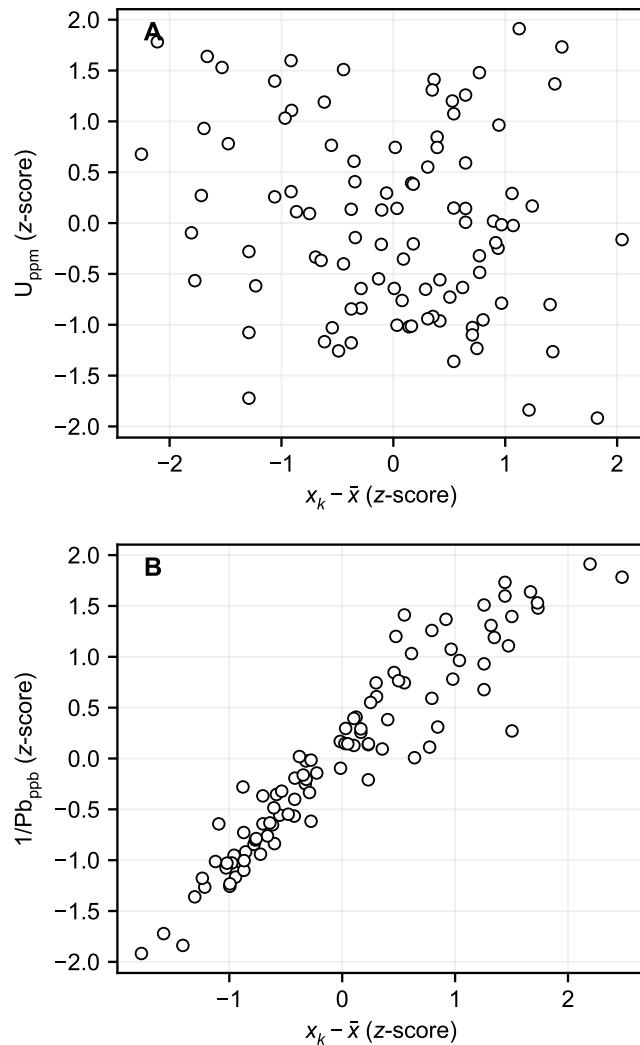


Figure S4. Dispersion of U–Pb data along the regression line plotted against U content (in ppm) and the reciprocal of total-Pb content (in ppb^{-1}). Data are plotted as a z -score to allow data points for all age samples to be plotted together and directly compared. Dispersion of data is calculated as the distance in x of the least-squares fitted data points (x_k) relative to the isochron centroid (\bar{x}). This clearly demonstrates that spread of data along the isochron is attributed mostly to variation in total-Pb content rather than U content. See Sect. 4.2 in the main text for further discussion.

S4 Speleothem $\delta^{238}\text{U}$ versus $[^{234}\text{U}/^{238}\text{U}]$

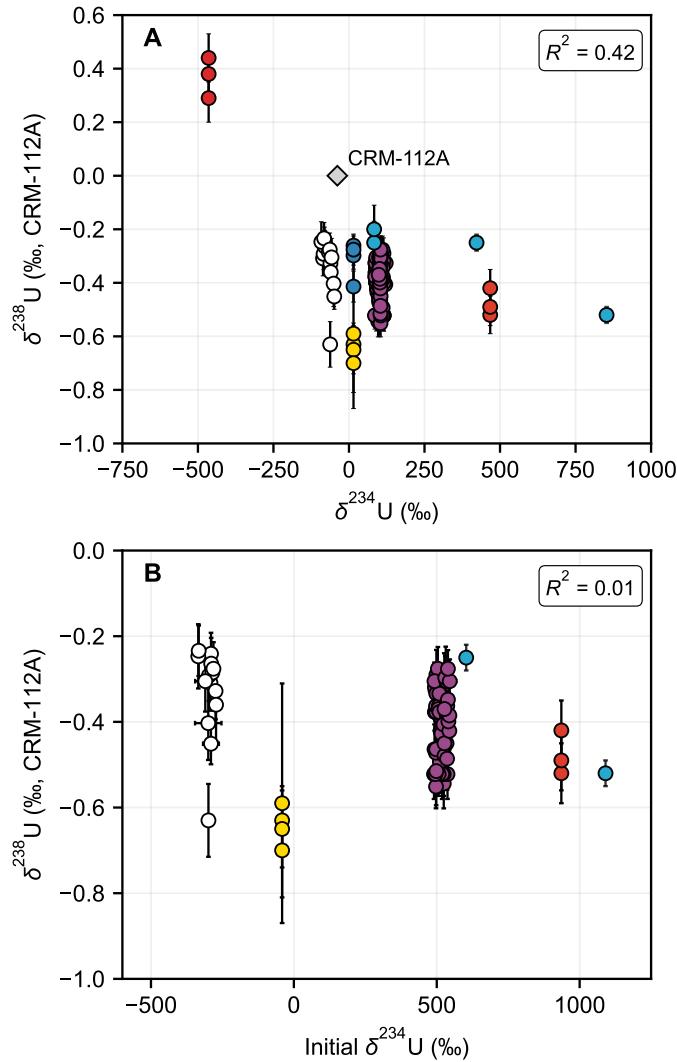


Figure S5. (A) Comparison of speleothem $\delta^{238}\text{U}$ and $\delta^{234}\text{U}$ values for the samples presented in Fig. 6. The coefficient of determination (R^2) is also provided. Where more than one measurement was available for an individual cave site, an average value was used to compute R^2 , in order to avoid biasing the results according to the number of analyses conducted for a particular site. Samples that are not analytically resolvable from secular equilibrium were excluded from the plot and R^2 calculation. CRM-112a is plotted for comparison but was not included in the R^2 calculation. (B) $\delta^{238}\text{U}$ plotted against initial $\delta^{234}\text{U}$ for speleothem samples where age data is available. Again, a sample average was used to compute R^2 in cases where analyses were made on multiple speleothems from the same site.

References

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