A. Linear least squares fitting of data

To fit a set of (x,y) data (*e.g.*, isotope ratio *vs.* time, or calibration material *vs.* time.) to an equation for a straight line: $y=a_1+a_2x$ find the values a_1 and a_2 which minimizes S, the sum of the squares of weighted deviation of a data points the fitted line. This is the fundamental principle of least squares analysis:

$$S = \sum (y_{data} - y_{calc})^2$$

Where y_{data} is the measured value and y_{calc} is the predicted y-value based on the fit of the data. In this equation and this derivation, the weight of each term in the above sum is constant, and effectively set to one. Other derivations can be made which for example set a weight of each term in the above sum to a relative constant, that is the relative uncertainties or standard deviations are constant. As well when uncertainty values are available for each term then these data uncertainity values can be used. Also implied in this derivation is that there is no uncertainty in the x values and the uncertainty in all of the y values s assumed to be constant. In cases where there is uncertainty in both x and y values the derivation becomes slightly more complicated as the two simultaneous equations which result do not lead to a direct solution, but instead an iterative solution is needed. For the purpose of this work, the assumption of constant uncertainty in the y data and no uncertainty in the x data is a very good assumption as explained in the main text.

Substituting for a *linear* least squares fit yields:

$$S = \sum (y_i - a_1 - a_2 x_i)^2$$

The principle of the least squares algorithm is to find the values of a_1 and a_2 which give the minimum value for S. The values for a_1 and a_2 are found by taking the partial derivative of S with respect to a_1 and a_2:

$$\frac{\partial S}{\partial a_1} = 2\sum (y_i - a_1 - a_2 x_i)(-1)$$
$$\frac{\partial S}{\partial a_2} = 2\sum (y_i - a_1 - a_2 x_i)(-x)$$

The partial derivatives are then set to zero and each equation divided by 2. This results in two simultaneous equations in the two unknowns a_1 and a_2:

$$\sum (y_i - a_1 - a_2 x_i)(-1) = 0$$

$$\sum (y_i - a_1 - a_2 x_i)(-x) = 0$$

Rearranging gives:

$$\sum(-y_i + a_1 + a_2 x_i) = 0$$

$$\sum(-xy_i + a_1 x + a_2 x^2) = 0$$

Further rearranging gives:

$$a_1 \sum 1 + a_2 \sum x = \sum y$$
$$a_1 \sum x + a_2 \sum x^2 = \sum xy$$

From the data the sums are calculated over all data points; Σy, Σxy, $\Sigma 1$, Σx, Σx^2. The sum $\Sigma 1$ is equal to "N" the number of data points.

These two simultaneous equations can be solved directly using substitution methods. Giving:

$$a_1 = \frac{\sum y \sum x^2 - \sum x \sum xy}{\sum 1 \sum x^2 - \left(\sum x^2\right)}$$

$$a_2 = \frac{\sum 1 \sum xy - \sum y \sum x}{\sum 1 \sum x^2 - \left(\sum x^2\right)}$$

Or as mentioned derivations usually substitute the number of data points, N, for the sum of one, which yields the following equations for a_1 and a_2:

$$a_1 = \frac{\sum y \sum x^2 - \sum x \sum xy}{N \sum x^2 - \left(\sum x^2\right)}$$

$$a_2 = \frac{N \sum xy - \sum y \sum x}{N \sum x^2 - \left(\sum x^2\right)}$$

The above solution for the adjustable parameters a_1 and a_2 does not conveniently lead to calculation of the uncertainty in these fitted parameters, and therefore the fitted or calculated values. Thus it is preferable to use matrix algebra to solve these two simultaneous equations.

A set of the two equations in matrix algebra notations is:

$$C * A = V$$

Where the C, A and V matrices are:

$$C = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} N & \sum x \\ \sum x & \sum x^2 \end{pmatrix}$$

$$A = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$$V = \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} \sum y \\ \sum xy \end{pmatrix}$$

The matrix equation is solved by multiplying both sides by the inverse matrix:

$$C^{-1} * C * A = A = C^{-1} * V$$

Where the inverse C matrix (C^{-1}) is:

$$\begin{pmatrix} C^{-1}_{11} & C^{-1}_{12} \\ C^{-1}_{21} & C^{-1}_{22} \end{pmatrix} = \begin{pmatrix} \frac{\sum x^2}{D} & \frac{-\sum x}{D} \\ \frac{-\sum x}{D} & \frac{N}{D} \end{pmatrix}$$

where, D, the determinate is given by:

$$D = C_{11} * C_{22} - C_{12} * C_{21}$$

$$\begin{pmatrix} C^{-1}_{11} & C^{-1}_{12} \\ C^{-1}_{21} & C^{-1}_{22} \end{pmatrix} * \begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

After calculating S, the sum of the squares of the deviations, the uncertainty of the adjustable parameters (a_1 and a_2) are calculated as:

$$\sigma^2_{a1} = s^2_1 = \frac{SC^{-1}_{11}}{N - p}$$

$$\sigma_{a2}^2 = s_2^2 = \frac{SC_{22}^{-1}}{N-p}$$

where S is the sum of the squares of weighted deviation of a calculated point from a fitted line, (n-p) is the number of degrees of freedom, with N being the number of data points, and p is the number of adjustable parameters, which in this case is equal to two.
The covariance is given by:

$$s_{12}^2 = \frac{SC_{12}^{-1}}{n-p}$$

Then, the uncertainty for each calculated y value which is a function of x is given by:

$$\sigma y = \sqrt{\sigma^2{}_{a1} + 2x\sigma^2{}_{12} + x^2\sigma^2{}_{a2}}$$

Substituting:

$$\sigma y = \sqrt{\frac{S}{n-p}\left(C_{11}^{-1} + 2xC_{12}^{-1} + x^2C_{22}^{-1}\right)}$$

B. Quadratic least squares fit

Any other equation can be fit, with the second most common equation being that of a quadratic which has three adjustable parameters. To fit a set of (x,y) data (*e.g.*, isotope ratio *vs.* time, or calibration material *vs.* time.) to the equation $y=a_1+a_2x+a_3x^2$ find the values a_1, a_2, and a_3 which minimizes S, the sum of the squares of the weighted deviation of a calculated point from a fitted line. As for the linear case:

$$S = \sum (y_{data} - y_{calc})^2$$

Where y_{data} is the measured value and y_{calc} is the predicted y-value based on the fit of the data. Rearranging for a *quadratic* least squares fit criteria yields:

$$S = \sum (y_i - a_1 - a_2x_i - a_3x^2)^2$$

The minimum value of S, which is the least squares criteria is found by taking the partial derivatives of S with respect to a_1, a_2, and a_3:

$$\frac{\partial S}{\partial a_1} = 2\sum (y_i - a_1 - a_2x_i - a_3x^2)(-1)$$
$$\frac{\partial S}{\partial a_2} = 2\sum (y_i - a_1 - a_2x_i - a_3x^2)(-x)$$

$$\frac{\partial S}{\partial a_2} = 2\sum (y_i - a_1 - a_2 x_i - a_3 x^2)(-x^2)$$

The partial derivatives are then set to zero:

$$\sum (y_i - a_1 - a_2 x_i - a_3 x^2)(-1) = 0$$

$$\sum (y_i - a_1 - a_2 x_i - a_3 x^2)(-x) = 0$$

$$\sum (y_i - a_1 - a_2 x_i - a_3 x^2)(-x^2) = 0$$

Multiplying and rearranging gives the following three simultaneous equations in three unknowns:

$$\sum (-y_i + a_1 + a_2 x_i) = 0$$

$$\sum (-x y_i + a_1 x + a_2 x^2 + a_3 x^2) = 0$$

$$\sum (-x^2 y_i + a_1 x^2 + a_2 x^3 + a_3 x^4) = 0$$

From the data the following sums are calculated for all data points; Σy, Σxy, $\Sigma x^2 y$,Σ1, Σx, Σx^2, Σx^3, Σx^4. Rearranging the three simultaneous equations gives:

$$\begin{aligned} a_1 \sum 1 + a_2 \sum x + a_3 \sum x^2 &= \sum y \\ a_1 \sum x + a_2 \sum x^2 + a_3 \sum x^3 &= \sum xy \\ a_1 \sum x^2 + a_2 \sum x^3 + a_3 \sum x^4 &= \sum x^2 y \end{aligned}$$

It is preferable and most convenient to solve these three simultaneous equations above using matrix algebra.

A set of two equations in matrix algebra notations is:

$$C * A = V$$

Where the C, A and V matrices are as follows:

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix} = \begin{pmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{pmatrix}$$

$$A = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$V = \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} = \begin{pmatrix} \sum y \\ \sum xy \\ \sum x^2 y \end{pmatrix}$$

This set of equations is solved by multiplying both sides by the inverse C matrix:

$$C^{-1} * C * A = A = C^{-1} * V$$

The inverse C matrix is found by:

$$C * C^{-1} = 1$$

expanding the above equation:

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix} * \begin{pmatrix} C^{-1}_{11} & C^{-1}_{12} & C^{-1}_{13} \\ C^{-1}_{21} & C^{-1}_{22} & C^{-1}_{23} \\ C^{-1}_{31} & C^{-1}_{32} & C^{-1}_{33} \end{pmatrix} = 1$$

Due to the symmetry of the inverse C matrix:

$$C_{12} = C_{21}; C_{13} = C_{31}; C_{23} = C_{32}$$

The elements of inverse C matrix can be calculated directly, again noting that the square matrices are symmetrical:

$$C^{-1}_{11} = \frac{C_{22}C_{33} - (C_{23})^2}{D} = \frac{\sum x_i^2 \sum x_i^4 - \left(\sum x_i^3\right)^2}{D}$$

$$C^{-1}_{22} = \frac{C_{11}C_{33} - (C_{13})^2}{D} = \frac{n\sum x_i^4 - \left(\sum x_i^2\right)^2}{D}$$

$$C^{-1}_{33} = \frac{C_{11}C_{22} - (C_{12})^2}{D} = \frac{n\sum x_i^2 - \left(\sum x_i\right)^2}{D}$$

$$C_{12}^{-1} = C_{21}^{-1} = \frac{C_{13}C_{23} - C_{12}C_{33}}{D} = \frac{\sum x_i^2 \sum x_i^3 - \sum x_i \sum x_i^4}{D}$$

$$C_{13}^{-1} = C_{31}^{-1} = \frac{C_{12}C_{23} - C_{13}C_{22}}{D} = \frac{\sum x_i \sum x_i^3 - \left(\sum x_i^2\right)^2}{D}$$

$$C_{23}^{-1} = C_{32}^{-1} = \frac{C_{12}C_{13} - C_{11}C_{23}}{D} = \frac{\sum x_i \sum x_i^2 - n\sum x_i^3}{D}$$

The determinate (D) is given by:

$$D = C_{11}\left(C_{22} * C_{33} - C_{23}C_{32}\right) - C_{12}\left(C_{12} * C_{33} - C_{13} * C_{23}\right) + C_{13}\left(C_{12} * C_{23} - C_{13} * C_{22}\right)$$

The adjustable parameters a1, a2, and a3 can be determined from C, A, and V matrices as follows:

$$C^{-1} * V = A$$

Expanding the above equation for the case of a quadratic fit yields:

$$\begin{pmatrix} C_{11}^{-1} & C_{12}^{-1} & C_{13}^{-1} \\ C_{21}^{-1} & C_{22}^{-1} & C_{23}^{-1} \\ C_{31}^{-1} & C_{32}^{-1} & C_{33}^{-1} \end{pmatrix} * \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

The equations for the adjustable parameters are as follows:

$$a_1 = C_{11}^{-1}V_1 + C_{12}^{-1}V_2 + C_{13}^{-1}V_3$$

$$a_2 = C_{21}^{-1}V_1 + C_{22}^{-1}V_2 + C_{23}^{-1}V_3$$

$$a_3 = C_{31}^{-1}V_1 + C_{32}^{-1}V_2 + C_{33}^{-1}V_3$$

The calculated values (y) as a function of x can be is determined as follows:

$$y = a_1 + a_2 x_i + a_3 x_i^2$$

The elements of the inverse C matrix are used to find the uncertainty in the adjustable parameters and therefore the uncertainty in the calculated y values. The uncertainty of the adjustable parameters a_1, a_2, and, a_3 is given by:

$$\sigma_{a1}^2 = s_1^2 = \frac{SC_{11}^{-1}}{N-p}$$

$$\sigma_{a2}^2 = s_2^2 = \frac{SC_{22}^{-1}}{N-p}$$

$$\sigma_{a3}^2 = s_2^2 = \frac{SC_{33}^{-1}}{N-p}$$

where S is the sum of the squares of weighted deviation of a calculated point from a fitted line, (N-p) is the number of degrees of freedom, with n being the number of data points, and p is the number of adjustable parameters, which in this case is three.

The covariances are given by:

$$s_{12}^2 = \frac{SC_{12}^{-1}}{n-p}$$

$$s_{13}^2 = \frac{SC_{13}^{-1}}{n-p}$$

$$s_{23}^2 = \frac{SC_{23}^{-1}}{n-p}$$

Finally, the uncertainty in the fit is given by the following equation:

$$\sigma y^2 = \sigma_{a1}^2 + x^2\sigma_{a2}^2 + x^4\sigma_{a3}^2 + 2xs_{12}^2 + 2x^2s_{13}^2 + 2x^3s_{23}^2$$

where the final three terms are the covariance terms.

Rewriting the above equation and expanding terms:

$$\sigma y = \sqrt{\frac{S}{N-2} * \left(C_{11}^{-1} + x_i^2 C_{22}^{-1} + x_i^3 C_{23}^{-1} + 2x_i C_{12}^{-1} + 2x_i^2 C_{13}^{-1} + 2x_i^3 C_{23}^{-1}\right)}$$

References:

Wolberg, J.R., Prediction Analysis, D. Van Nostrand, Inc., Princeton, New Jersey, 291 pp.

C. Summary of U-Pb isotopic data for the 91500 and Plešovice zircons

Summary of results for 91500

		Linear-MOR			Quadratic			Mean- standard error[a]			Mean- standard deviation[b]		
	Mean of Ratios (MOR)	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**
1, 2, 3, 18, 19, 20	weighted mean age[c]	1057.1	1060.7	1068.9	1080.4	1078.8	1091.2	1059.4	1063.3	1069.5	1059.7	1064.4	1068.7
	MSWD[d]	8.00	5.50	1.40	3.40	4.00	1.40	2.60	2.80	1.09	0.57	0.67	0.53
	mean 2RSE%[e]	1.45	1.19	2.56	3.32	2.17	4.33	2.21	1.51	2.56	4.73	2.99	3.66
	2RSD% age[f]	4.34	3.04	2.95	2.61	0.99	2.33	4.41	3.18	2.56	4.41	3.18	2.66
	Coverage[g]	2.85	2.37	1.16	1.85	1.18	1.20	1.62	1.70	1.05	0.76	0.82	0.73
	recalculated mean 2RSE%[h]	4.12	2.78	2.97	4.81	2.54	5.60	3.58	2.53	2.68	3.59	2.44	2.67
	recalcuated MSWD[i]	0.99	1.00	1.01	1.00	1.00	1.01	1.00	0.99	0.99	0.99	1.01	0.99
1, 2, 10, 11, 19, 20	weighted mean age[c]	1057.5	1060.2	1066.4	1056.9	1059.1	1068.4	1058.2	1061.2	1066.9	1058.3	1062.4	1065.0
	MSWD[d]	3.40	2.00	1.80	2.6	1.80	2.20	2.10	1.80	1.80	0.70	0.50	1.08
	mean 2RSE%[e]	1.75	1.46	2.57	1.28	1.12	1.31	2.18	1.57	2.49	4.54	3.16	3.34
	2RSD% age[f]	3.71	2.36	3.35	2.18	1.53	3.74	3.81	2.48	3.29	3.81	2.48	3.29
	Coverage[g]	1.84	1.44	1.34	1.60	1.35	1.50	1.45	1.33	1.34	0.83	0.71	1.03
	recalculated mean 2RSE%[h]	3.21	2.09	3.44	2.05	1.51	3.94	3.15	2.07	3.34	3.76	2.33	3.44
	recalcuated MSWD[i]	1.01	0.99	1.01	1.01	0.98	0.99	1.02	1.02	1.01	1.02	1.00	1.02
Every other	weighted mean age[c]	1063.7	1063.8	1064.9	1064.6	1064.7	1064.7	1063.8	1064.5	1064.9	1063.5	1065.1	1064.6
	MSWD[d]	1.90	2.20	0.97	1.70	1.60	1.60	2.90	2.90	1.09	0.54	0.61	0.45
	mean 2RSE%[e]	1.68	1.21	2.65	1.31	1.05	1.38	1.60	1.17	2.48	3.88	2.59	3.88
	2RSD% age[f]	2.76	2.09	2.55	1.75	1.25	2.81	3.41	2.42	2.53	3.41	2.42	2.53
	Coverage[g]	1.39	1.50	0.97	1.32	1.25	1.05	1.70	1.72	1.04	0.74	0.78	0.67
	recalculated mean 2RSE%[h]	2.33	1.81	2.57	1.73	1.31	2.90	2.71	2.00	2.58	2.87	2.01	2.60
	recalcuated MSWD[i]	1.01	1.00	1.00	1.00	1.00	1.00	1.01	1.01	1.01	0.99	1.02	1.00
Adjacent	weighted mean age[c]	1065.1	1065.4	1065.7									
	MSWD[d]	1.70	1.60	1.30									
	mean 2RSE%[e]	1.37	1.70	1.49									
	2RSD% age[f]	1.73	2.11	1.71									
	Coverage[g]	1.33	1.27	1.15									
	recalculated mean 2RSE%[h]	1.67	1.33	3.24									
	recalcuated MSWD[i]	0.99	1.00	0.99									

	Ratio of Means (ROM)	Linear-MOR			Quadratic			Mean- standard error[a]			Mean- standard deviation[b]		
		$^{206}Pb/^{238}U$	$^{207}Pb/^{235}U$	$^{207}Pb/^{206}Pb$	$^{206}Pb/^{238}U$	$^{207}Pb/^{235}U$	$^{207}Pb/^{206}Pb$	$^{206}Pb/^{238}U$	$^{207}Pb/^{235}U$	$^{207}Pb/^{206}Pb$	$^{206}Pb/^{238}U$	$^{207}Pb/^{235}U$	$^{207}Pb/^{206}Pb$
1, 2, 3, 18, 19, 20	weighted mean age[c]	1056.2	1059..8	1069.6	1077.8	1080.9	1094.1	1062.6	1064.4	1068.8	1063.1	1065.9	1068.0
	MSWD[d]	8.10	4.70	1.30	2.70	0.91	1.50	2.10	2.10	0.95	0.56	0.67	0.47
	mean 2RSE%[e]	1.45	1.19	2.56	2.53	2.34	2.37	2.22	1.62	2.77	4.34	2.77	3.89
	2RSD% age[f]	4.24	2.98	2.95	2.83	1.84	4.15	3.57	2.61	2.60	3.57	2.61	2.60
	Coverage[g]	2.85	2.37	1.16	1.65	0.95	1.20	1.45	1.45	0.98	0.76	0.82	0.69
	recalculated mean 2RSE%[h]	4.12	2.78	2.97	4.17	2.21	5.68	3.21	2.33	2.72	3.29	2.26	2.68
	recalcuated MSWD[i]	0.99	1.00	1.01	0.99	1.01	1.01	1.00	1.00	0.99	0.98	1.01	0.98
1, 2, 10, 11, 19, 20	weighted mean age[c]	1057.4	1060.1	1067.8	1056.7	1060.2	1069.7	1058.3	1061.0	1068.2	1058.2	1062.2	1066.1
	MSWD[d]	3.40	1.60	1.60	2.50	1.08	2.10	2.20	1.50	1.70	0.78	0.45	1.01
	mean 2RSE%[e]	1.73	1.62	2.72	1.32	1.33	1.39	2.18	1.73	2.63	4.45	3.24	3.46
	2RSD% age[f]	3.61	2.27	3.32	2.14	1.42	3.76	3.78	2.45	3.27	3.78	2.45	3.27
	Coverage[g]	1.86	1.27	1.28	1.58	1.05	1.45	1.50	1.22	1.30	0.88	0.68	1.01
	recalculated mean 2RSE%[h]	3.22	2.05	3.48	2.09	1.40	4.03	3.26	2.10	3.42	3.91	2.19	3.52
	recalcuated MSWD[i]	0.99	1.01	1.01	0.99	0.99	0.98	0.99	1.01	0.99	1.01	0.99	0.99
Every other	weighted mean age[c]	1064.0	1064.1	1066.3	1064.9	1065.4	1065.7	1064.2	1064.9	1066.4	1064.1	1065.4	1065.8
	MSWD[d]	1.80	1.60	0.83	1.60	0.97	1.01	2.90	2.50	0.94	0.58	0.57	0.43
	mean 2RSE%[e]	1.72	1.41	2.79	1.36	1.25	1.44	1.64	1.37	2.64	3.83	2.66	3.87
	2RSD% age[f]	2.69	2.02	2.46	1.72	1.18	2.71	3.43	2.41	2.44	3.43	2.41	2.44
	Coverage[g]	1.34	1.29	0.91	1.25	0.99	1.00	1.70	1.60	0.96	0.76	0.76	0.65
	recalculated mean 2RSE%[h]	2.30	1.81	2.54	1.70	1.24	2.89	2.78	2.18	2.53	2.91	2.10	2.52
	recalcuated MSWD[i]	1.00	0.99	1.01	1.02	1.00	1.01	1.01	0.98	1.02	1.01	1.00	1.02
Adjacent	weighted mean age[c]	1065.2	1065.7	1066.8									
	MSWD[d]	1.60	1.01	1.14									
	mean 2RSE%[e]	1.34	1.34	1.51									
	2RSD% age[f]	1.56	1.28	3.16									
	Coverage[g]	1.25	1.00	1.07									
	recalculated mean 2RSE%[h]	1.68	1.34	3.23									
	recalcuated MSWD[i]	1.00	1.02	0.99									

		Linear-MOR			Quadratic			Mean- standard error[a]			Mean- standard deviation[b]		
	Intercept (INTC)	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**
1, 2, 3, 18, 19, 20	weighted mean age[c]	1051.9	1057.9	1068.9	1062.8	1081.8	1091.2	1059.9	1060.8	1069.5	1062.7	1062.3	1068.7
	MSWD[d]	5.30	2.90	1.40	0.75	0.38	1.40	2.30	2.60	1.09	0.70	0.87	0.53
	mean 2RSE%[e]	2.20	2.21	2.56	5.03	5.26	4.66	3.04	2.35	2.56	5.81	4.03	3.66
	2RSD% age[f]	4.61	3.65	2.95	4.51	2.75	4.33	4.80	3.91	2.66	4.80	3.91	2.66
	Coverage[g]	2.30	1.75	1.16	0.86	0.62	1.20	1.52	1.65	1.04	0.83	0.93	0.72
	recalculated mean 2RSE%[h]	5.05	3.81	2.97	4.32	3.25	5.60	4.61	3.82	2.66	4.82	3.72	2.64
	recalcuated MSWD[i]	1.00	0.99	1.01	1.01	0.99	1.01	1.00	1.00	1.01	1.02	1.02	1.02
1, 2, 10, 11, 19, 20	weighted mean age[c]	1056.8	1063.7	1077.5	1056.7	1060.2	1068.4	1059.1	1064.2	1076.8	1061.1	1064.7	1076.5
	MSWD[d]	2.80	1.30	0.82	2.50	1.08	2.20	2.30	1.70	0.86	0.80	0.58	0.39
	mean 2RSE%[e]	2.47	2.60	6.12	2.41	2.59	1.31	2.91	2.49	5.72	5.38	4.45	8.52
	2RSD% age[f]	4.02	2.94	5.44	3.40	2.63	3.74	4.48	3.32	5.16	4.48	3.22	5.16
	Coverage[g]	1.68	1.16	0.90	1.40	1.05	1.50	1.52	1.30	0.93	0.90	0.76	0.62
	recalculated mean 2RSE%[h]	4.13	2.99	5.51	3.37	2.70	3.94	4.41	3.20	5.32	4.83	3.36	5.28
	recalcuated MSWD[i]	0.99	1.00	1.01	1.01	0.98	0.99	1.02	1.02	0.99	0.99	1.01	1.01
Every other	weighted mean age[c]	1063.3	1066.7	1064.7	1064.5	1066.6	1064.6	1064.0	1066.9	1064.9	1066.4	1068.6	1064.6
	MSWD[d]	2.40	2.70	0.95	1.70	2.10	1.11	3.90	2.90	1.09	0.84	0.88	0.45
	mean 2RSE%[e]	2.48	2.18	2.65	2.37	2.11	1.38	2.39	2.09	2.48	4.75	3.83	3.88
	2RSD% age[f]	3.82	3.62	2.55	3.06	3.08	2.81	4.76	3.59	2.53	4.76	3.59	2.53
	Coverage[g]	1.55	1.65	0.97	1.32	1.45	1.05	1.92	1.72	1.04	0.91	0.94	0.67
	recalculated mean 2RSE%[h]	3.84	3.55	2.57	3.12	3.03	2.90	4.58	3.54	2.58	4.32	3.56	2.60
	recalcuated MSWD[i]	0.99	1.01	1.00	0.99	1.01	1.00	1.02	1.01	1.01	1.02	1.02	1.00
Adjacent	weighted mean age[c]	1064.3	1066.3	1065.7									
	MSWD[d]	1.19	2.20	1.30									
	mean 2RSE%[e]	2.47	2.22	1.41									
	2RSD% age[f]	2.69	3.39	3.23									
	Coverage[g]	1.10	1.50	1.15									
	recalculated mean 2RSE%[h]	2.71	3.30	3.24									
	recalcuated MSWD[i]	0.98	1.02	0.99									

[a] uncertainty of calibration based on standard error of calibration materials. [b] uncertainty of calibration based on standard error of calibration materials. [c] weighted mean of unknowns.
[d] MSWD of all unknowns before adjusting uncertainty (see text for further details). [e] mean 2 relative standard error of unknowns. [f] 2 relative standard deviation of calculated age
[g] coverage factor required to yield MSWD=1 for all unknowns (see text for further details). [h] recalculated mean 2 relative standard error after application of coverage factor.
[i] recalculated MSWD.

Summary of results for Plešovice

		Linear-MOR			Quadratic			Mean- standard error[a]			Mean- standard deviation[b]		
	Mean of Ratios (MOR)	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**
1, 2, 3, 18, 19, 20	weighted mean age[c]	334.3	333.6	328.3	334.9	334.5	326.3	334.3	333.1	329.5	334.2	333.0	332.9
	MSWD[d]	6.70	5.20	3.10	1.10	0.82	0.81	4.00	3.10	2.50	0.95	0.72	1.10
	mean 2RSE%[e]	1.61	1.74	7.52	5.76	6.34	9.05	2.12	2.28	7.83	4.65	5.05	13.04
	2RSD% age[f]	3.87	3.72	13.00	5.30	6.00	15.08	3.73	3.34	12.16	3.73	3.43	12.16
	Coverage[g]	2.60	2.28	1.77	1.05	0.90	0.90	2.00	1.75	1.60	0.98	0.85	1.04
	recalculated mean 2RSE%[h]	4.18	3.94	13.31	6.00	5.70	16.28	4.23	3.96	12.53	4.56	4.28	13.56
	recalcuated MSWD[i]	0.99	1.00	1.00	1.00	1.02	1.00	1.01	1.01	1.01	0.99	1.00	1.01
1, 2, 10, 11, 19, 20	weighted mean age[c]	335.1	333.3	324.4	335.2	334.1	325.2	335.6	334.9	327.8	335.8	335.0	330.4
	MSWD[d]	7.80	9.40	2.90	8.2	12.00	3.40	2.60	2.30	1.70	0.58	0.50	0.56
	mean 2RSE%[e]	1.61	1.63	7.97	1.57	1.42	3.88	2.19	2.34	8.25	4.86	5.24	14.62
	2RSD% age[f]	4.04	4.19	13.31	4.11	4.31	12.69	3.32	3.18	10.97	3.32	3.18	10.97
	Coverage[g]	2.78	3.10	1.72	2.90	3.45	1.85	1.60	1.50	1.30	0.76	0.70	0.75
	recalculated mean 2RSE%[h]	4.47	5.03	13.71	4.56	4.87	14.34	3.50	3.49	10.73	3.69	3.66	10.96
	recalcuated MSWD[i]	1.01	0.99	0.99	0.98	1.02	0.99	1.01	1.01	0.99	1.01	1.02	1.00
Every other	weighted mean age[c]	336.8	336.7	334.9	336.9	337.0	335.1	336.8	336.9	336.2	337.2	337.3	335.4
	MSWD[d]	4.80	4.00	0.94	3.30	2.70	0.96	7.00	6.70	1.70	1.19	1.12	0.39
	mean 2RSE%[e]	1.59	1.63	7.95	1.77	1.75	4.20	1.44	1.47	7.09	3.62	3.80	13.68
	2RSD% age[f]	3.49	3.27	7.86	3.23	3.00	8.32	4.04	3.94	8.32	4.04	3.94	8.32
	Coverage[g]	2.20	2.00	0.97	1.80	1.65	0.98	2.65	2.60	1.30	1.10	1.05	0.60
	recalculated mean 2RSE%[h]	3.50	3.24	7.71	3.18	2.88	8.24	3.82	3.81	9.22	3.97	3.85	8.21
	recalcuated MSWD[i]	0.99	1.02	0.99	1.01	1.00	0.99	1.00	1.00	1.00	0.99	1.02	1.02
Adjacent	weighted mean age[c]	337.5	336.9	335.6									
	MSWD[d]	2.20	3.10	2.30									
	mean 2RSE%[e]	1.20	1.23	3.65									
	2RSD% age[f]	2.59	2.39	10.52									
	Coverage[g]	2.00	1.87	1.55									
	recalculated mean 2RSE%[h]	2.40	2.18	11.32									
	recalcuated MSWD[i]	0.99	1.00	0.98									

	Ratio of Means (ROM)	Linear-MOR $^{206}Pb/^{238}U$	Linear-MOR $^{207}Pb/^{235}U$	Linear-MOR $^{207}Pb/^{206}Pb$	Quadratic $^{206}Pb/^{238}U$	Quadratic $^{207}Pb/^{235}U$	Quadratic $^{207}Pb/^{206}Pb$	Mean- standard error[a] $^{206}Pb/^{238}U$	Mean- standard error[a] $^{207}Pb/^{235}U$	Mean- standard error[a] $^{207}Pb/^{206}Pb$	Mean- standard deviation[b] $^{206}Pb/^{238}U$	Mean- standard deviation[b] $^{207}Pb/^{235}U$	Mean- standard deviation[b] $^{207}Pb/^{206}Pb$
1, 2, 3, 18, 19, 20	weighted mean age[c]	334.4	333.7	328.6	335.2	334.4	326.7	334.0	332.8	328.5	334.1	332.8	332.1
	MSWD[d]	6.40	4.10	2.90	0.98	0.72	0.79	2.70	1.80	2.40	0.68	0.48	1.50
	mean 2RSE%[e]	1.63	1.85	7.59	5.79	6.44	8.87	2.24	2.47	8.32	4.55	4.96	13.01
	2RSD% age[f]	3.88	3.64	12.88	5.37	5.91	14.13	3.41	2.99	12.46	3.41	2.99	12.46
	Coverage[g]	2.55	2.05	1.70	1.00	0.85	0.89	1.62	1.33	1.58	0.82	0.70	1.22
	recalculated mean 2RSE%[h]	4.15	3.78	12.90	5.79	5.45	15.79	3.62	3.27	13.15	3.73	3.47	15.87
	recalcuated MSWD[i]	0.99	0.99	1.01	0.99	1.00	0.99	1.01	1.00	0.98	1.01	0.98	1.02
1, 2, 10, 11, 19, 20	weighted mean age[c]	335.1	333.5	325.9	334.9	334.2	327.5	335.4	334.7	328.5	335.6	334.9	330.9
	MSWD[d]	6.90	7.60	2.50	7.00	8.90	3.00	2.50	1.90	1.50	0.55	0.45	0.53
	mean 2RSE%[e]	1.66	1.74	8.13	1.65	1.55	3.90	2.19	2.40	8.39	4.82	5.24	14.72
	2RSD% age[f]	4.00	4.11	13.01	3.99	4.16	12.49	3.26	3.08	10.62	3.26	3.08	10.62
	Coverage[g]	2.63	2.75	1.58	2.65	3.00	1.75	1.60	1.40	1.23	0.74	0.67	0.72
	recalculated mean 2RSE%[h]	4.36	4.75	12.85	4.36	4.62	13.64	3.50	3.35	10.32	3.57	3.50	10.66
	recalcuated MSWD[i]	1.00	1.01	1.00	0.99	1.00	0.98	0.97	0.97	0.99	1.01	1.00	1.01
Every other	weighted mean age[c]	336.8	336.9	335.2	336.9	337.1	335.5	336.9	336.9	336.3	337.2	337.3	335.6
	MSWD[d]	4.60	3.40	0.89	3.10	2.30	0.88	6.80	5.70	1.60	1.14	1.08	0.36
	mean 2RSE%[e]	1.61	1.71	7.94	1.77	1.83	4.20	1.45	1.57	7.11	3.60	3.67	13.60
	2RSD% age[f]	3.14	3.18	7.72	3.11	2.87	7.95	3.92	3.83	8.24	3.92	3.83	8.24
	Coverage[g]	2.16	1.86	0.95	1.75	1.50	0.95	2.40	1.26	2.10	1.06	1.04	0.60
	recalculated mean 2RSE%[h]	3.47	3.17	7.54	3.10	2.73	7.94	3.83	3.75	8.96	3.82	3.80	8.16
	recalcuated MSWD[i]	0.99	1.00	0.99	1.01	1.02	0.98	0.98	1.01	1.02	1.01	1.00	1.00
Adjacent	weighted mean age[c]	337.2	337.2	335.5									
	MSWD[d]	3.80	2.20	2.10									
	mean 2RSE%[e]	1.23	1.43	3.71									
	2RSD% age[f]	2.46	2.21	10.16									
	Coverage[g]	1.95	1.48	1.45									
	recalculated mean 2RSE%[h]	2.41	2.11	10.75									
	recalcuated MSWD[i]	0.48	0.48	0.47									

		Linear-MOR			Quadratic			Mean- standard error[a]			Mean- standard deviation[b]		
	Intercept (INTC)	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**	**$^{206}Pb/^{238}U$**	**$^{207}Pb/^{235}U$**	**$^{207}Pb/^{206}Pb$**
1, 2, 3, 18, 19, 20	weighted mean age[c]	337.0	336.6	328.3	340.1	338.6	326.3	336.9	336.2	329.5	338.2	336.2	332.9
	MSWD[d]	10.70	6.30	3.10	3.20	1.40	0.81	6.40	3.50	2.50	1.70	0.86	1.10
	mean 2RSE%[e]	2.33	2.56	7.52	5.87	6.85	9.05	3.13	3.48	7.83	6.29	7.07	13.04
	2RSD% age[f]	7.50	6.02	13.00	9.03	7.22	15.08	7.58	6.19	12.16	7.58	6.19	12.16
	Coverage[g]	3.26	2.55	1.77	1.80	1.20	0.90	2.50	1.88	1.60	1.30	0.93	1.04
	recalculated mean 2RSE%[h]	7.57	6.48	13.31	10.53	8.14	16.28	7.80	6.48	12.53	8.17	6.55	13.56
	recalcuated MSWD[i]	1.01	0.99	1.00	1.00	1.01	1.00	1.00	1.00	0.99	1.00	1.01	1.01
1, 2, 10, 11, 19, 20	weighted mean age[c]	335.8	336.9	338.7	334.5	336.5	325.2	335.6	336.0	339.3	336.1	336.9	334.0
	MSWD[d]	2.40	2.30	1.60	1.90	2.80	3.40	2.50	1.90	1.20	0.56	0.44	0.58
	mean 2RSE%[e]	3.94	3.40	14.47	4.51	3.31	3.88	3.78	3.74	14.87	8.20	7.85	22.11
	2RSD% age[f]	5.85	5.08	17.85	5.75	5.24	12.69	5.81	4.96	16.08	5.81	4.96	16.08
	Coverage[g]	1.54	1.50	1.28	1.37	1.70	1.85	1.40	1.10	2.10	0.75	0.67	0.76
	recalculated mean 2RSE%[h]	6.06	5.07	18.53	5.67	5.59	14.34	5.86	5.20	16.35	6.15	5.24	16.80
	recalcuated MSWD[i]	1.00	1.01	1.00	1.00	0.99	0.99	1.03	0.98	0.99	1.00	0.99	1.01
Every other	weighted mean age[c]	335.4	336.6	334.9	335.2	336.7	335.1	335.1	336.3	336.2	336.0	337.0	335.4
	MSWD[d]	3.9	3.2	4.7	2.70	2.20	0.96	6.50	5.60	1.70	1.17	1.20	0.37
	mean 2RSE%[e]	0.0	0.0	0.0	3.19	2.89	4.20	2.63	2.61	7.09	6.30	5.57	13.68
	2RSD% age[f]	2.99	2.79	7.95	5.36	4.49	8.32	6.84	6.23	8.32	6.84	6.23	8.32
	Coverage[g]	6.24	5.25	7.86	1.65	1.50	0.98	2.55	2.40	1.30	1.08	1.11	0.60
	recalculated mean 2RSE%[h]	2.20	1.90	0.97	5.26	4.32	8.24	6.68	6.20	9.22	6.80	6.14	8.21
	recalcuated MSWD[i]	6.58	5.27	7.71	0.98	0.99	0.99	1.00	1.00	1.00	1.01	1.02	1.02
Adjacent	weighted mean age[c]	336.2	336.9	335.6									
	MSWD[d]	4.40	2.20	2.30									
	mean 2RSE%[e]	2.31	2.54	3.65									
	2RSD% age[f]	4.98	3.90	10.52									
	Coverage[g]	2.10	1.47	1.54									
	recalculated mean 2RSE%[h]	4.85	3.72	11.25									
	recalcuated MSWD[i]	0.99	1.02	0.99									

[a] uncertainty of calibration based on standard error of calibration materials. [b] uncertainty of calibration based on standard error of calibration materials. [c] weighted mean of unknowns.
[d] MSWD of all unknowns before adjusting uncertainty (see text for further details). [e] mean 2 relative standard error of unknowns. [f] 2 relative standard deviation of calculated age
[g] coverage factor required to yield MSWD=1 for all unknowns (see text for further details). [h] recalculated mean 2 relative standard error after application of coverage factor.
[i] recalculated MSWD.