
CLIPPER

Evaluation of U-Pb laser ablation ICPMS data reduction software: an inter-laboratory comparison

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The Initiative

- To determine best practices in LA-ICP-MS U-Pb data processing
- Provide a set of (reasonably) standardized procedures
- Publish these as a paper(s) in a thematic issue

Software Evaluation

- Software comparison proposed at Charleston Workshop, 2013.
- Aims to evaluate & improve existing data-reduction packages
- Develop and distribute real data sets to developers and users of various software packages
  - 30 analyses of unknown zircon Z9910, previously dated by ID-TIMS at the GSC
  - Analysed in 5 blocks of 6 analyses with interspersed analyses of 91500 (14) for calibration, and GJ-1 (5) and Temora2 (5) as secondary standards

Instrumentation and Conditions

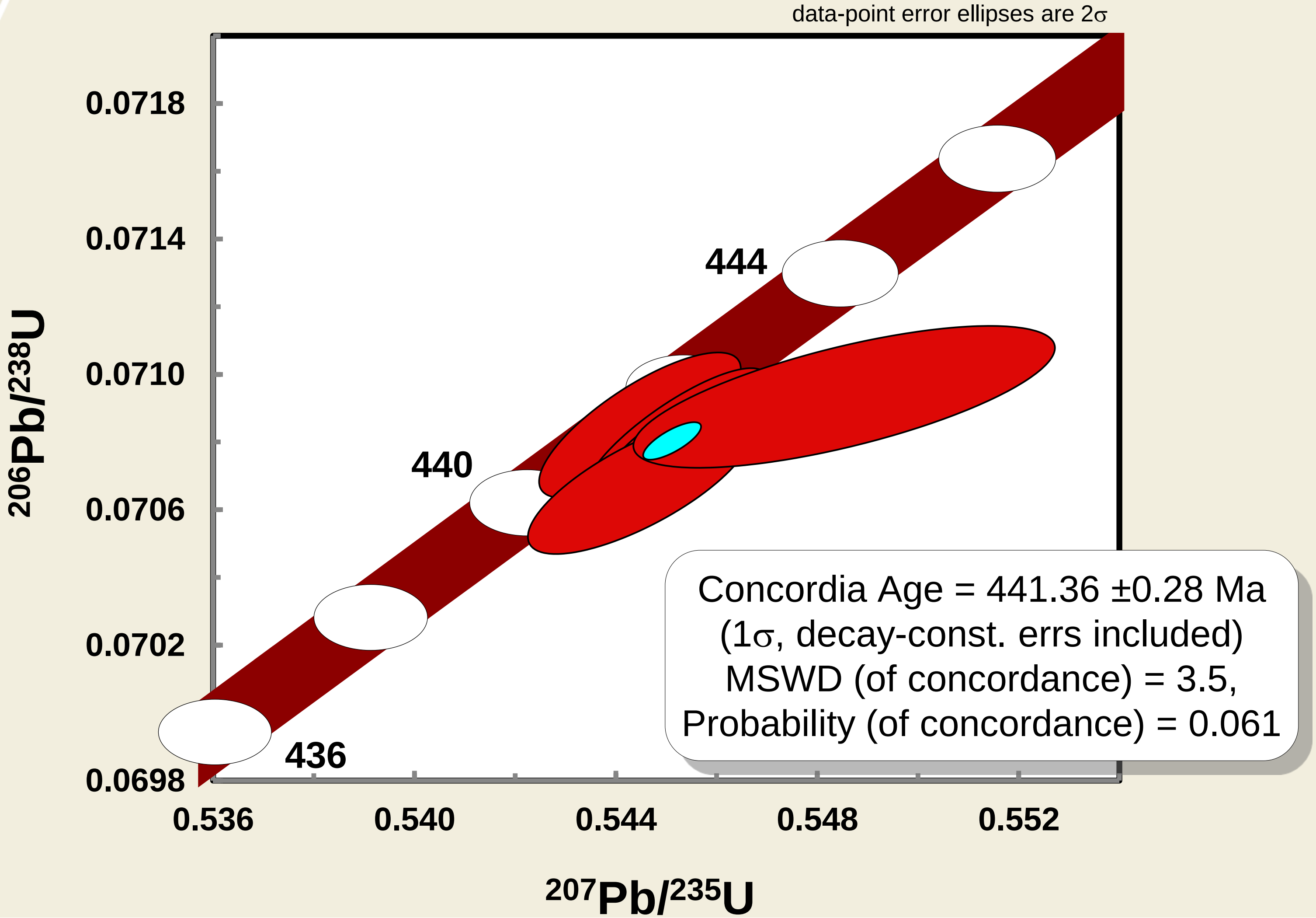
Parameter	Conditions
Laser Ablation system	Photon Machines Analyte.193
Sample cell	Helex 2-volume (99% washout in <0.7s)
ICP-MS	Agilent 7700 (Q) with additional interface pump
Spot size	34 µm
Rep rate	5 Hz
Gas blank	30 s
Ablation	60 s
Element list (dwell time in ms)	^{27}Al(1), ^{29}Si(5), ^{88}Sr(5), ^{96}Zr(5), ^{202}Hg(20), ^{204}Pb(20), ^{206}Pb(15), ^{207}Pb(50), ^{208}Pb(10), ^{232}Th(10), ^{238}U(10)
Total acquisition time	100 s

Zircon Z9910 ID-TIMS data

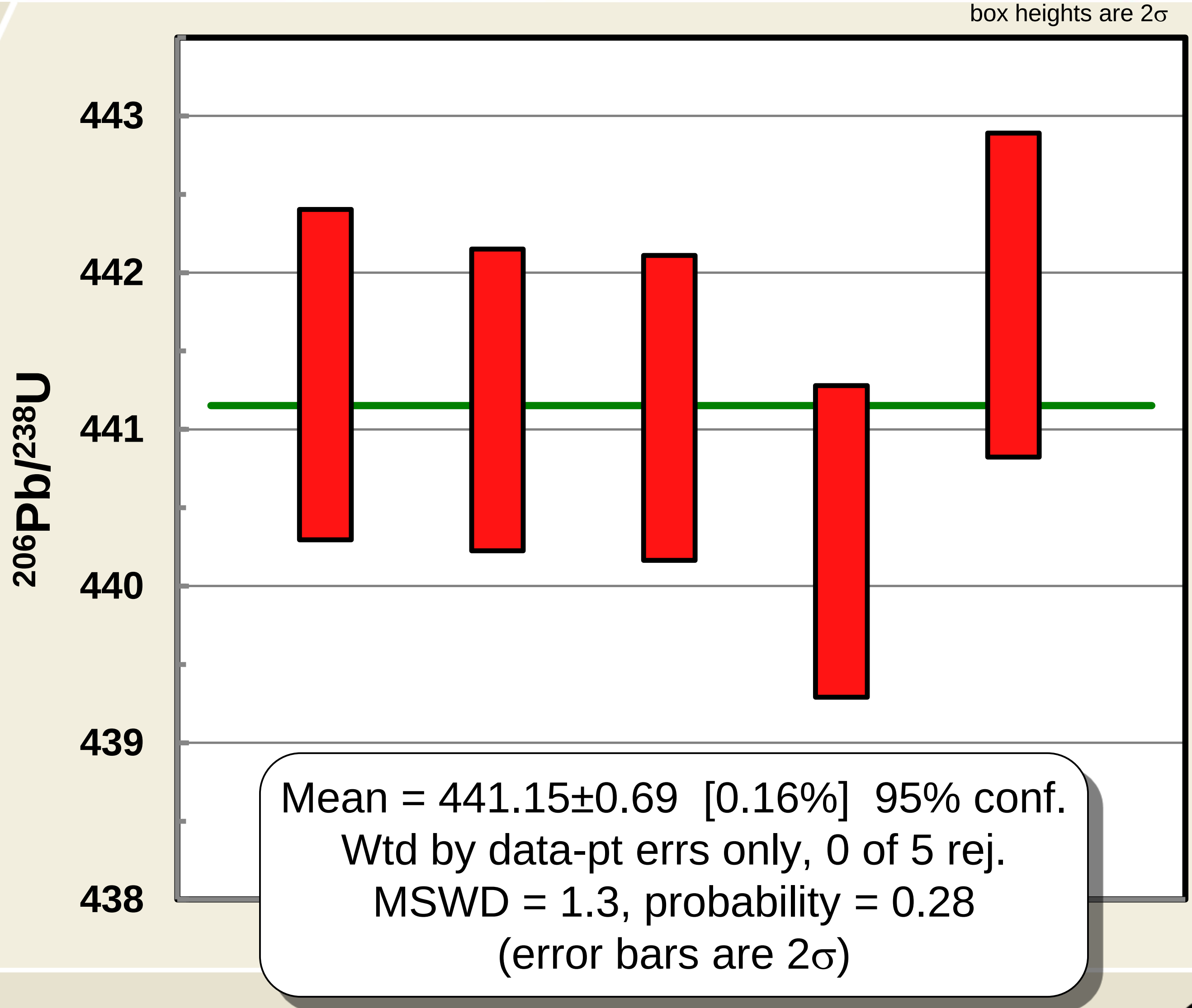
Fraction	Wt. ug	U ppm	Pb[1] ppm	206Pb[2] / 204Pb	Pb[3] pg	Isotopic Ratios[4] 208Pb / 206Pb	207Pb / 235U	±1SE Abs	206Pb / 238U	±1SE Abs	Corr.[5] Coeff.	207Pb / 206Pb	±1SE Abs
08-SNB-T170A (Z9910)													
A1 (Z)	15	85	7	3779	1.5	0.22	0.54459	0.00080	0.07086	0.00009	0.78	0.05574	0.00005
A2 (Z)	12	144	11	5736	1.3	0.21	0.54529	0.00072	0.07084	0.00008	0.82	0.05583	0.00004
A4 (Z)	7	162	12	2691	1.9	0.21	0.54579	0.00081	0.07083	0.00008	0.76	0.05589	0.00005
A5 (Z)	7	76	6	2837	0.8	0.20	0.54458	0.00089	0.07069	0.00008	0.75	0.05587	0.00006
A6 (Z)	9	77	6	590	5.2	0.24	0.54856	0.00167	0.07095	0.00008	0.69	0.05608	0.00013

Fraction	Ages (Ma)[6] 206Pb / 238U	±2SE	207Pb / 235U	±2SE	207Pb / 206Pb	±2SE	% Disc
08-SNB-T170A (Z9910)							
A1 (Z)	441.4	1.0	441.4	1.1	441.9	4.1	0.1
A2 (Z)	441.2	1.0	441.9	1.0	445.7	3.3	1.0
A4 (Z)	441.1	1.0	442.2	1.1	448.0	4.3	1.6
A5 (Z)	440.3	1.0	441.4	1.2	447.4	4.8	1.6
A6 (Z)	441.9	1.0	444.1	2.2	455.5	10.5	3.1

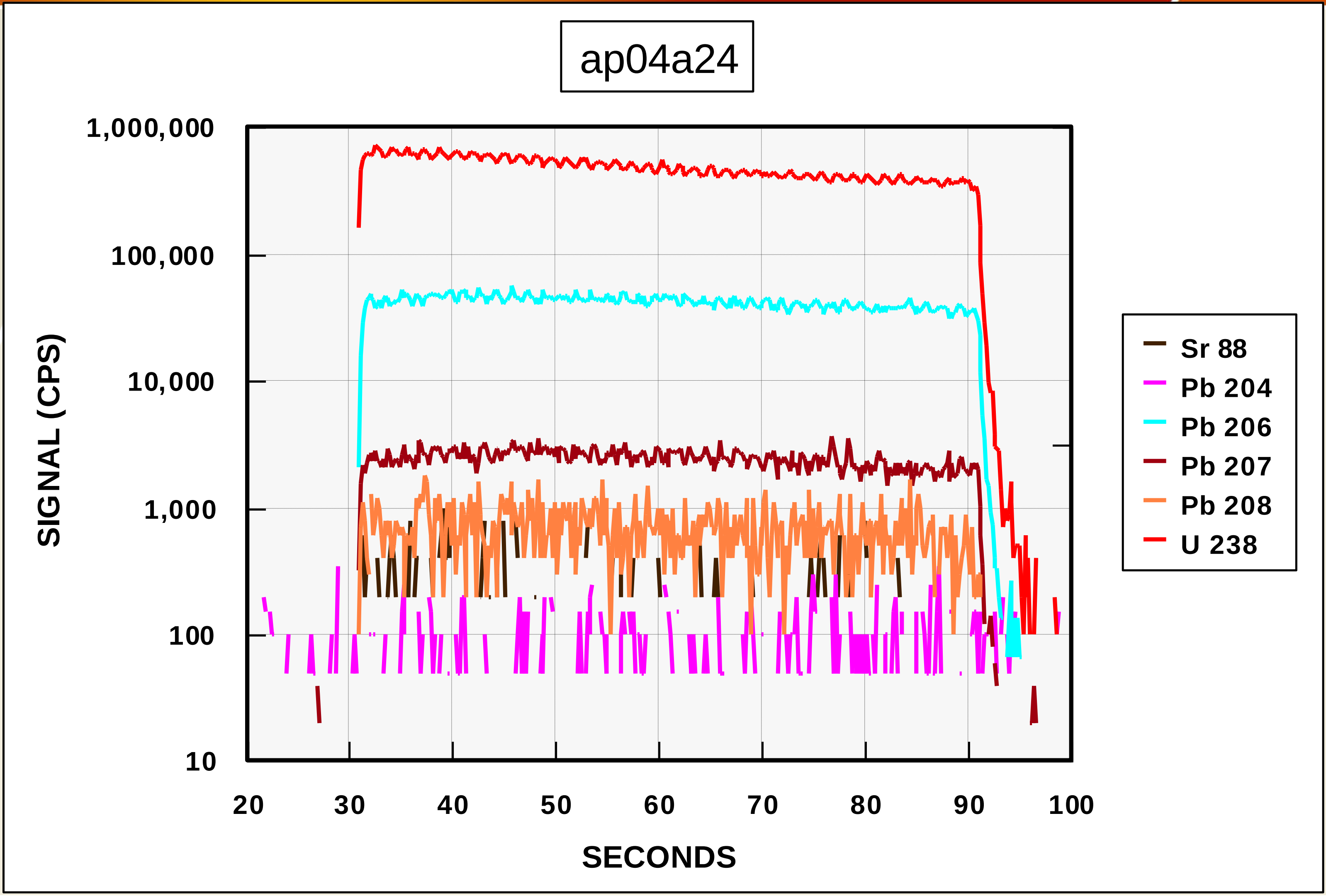
Zircon Z9910 ID-TIMS data



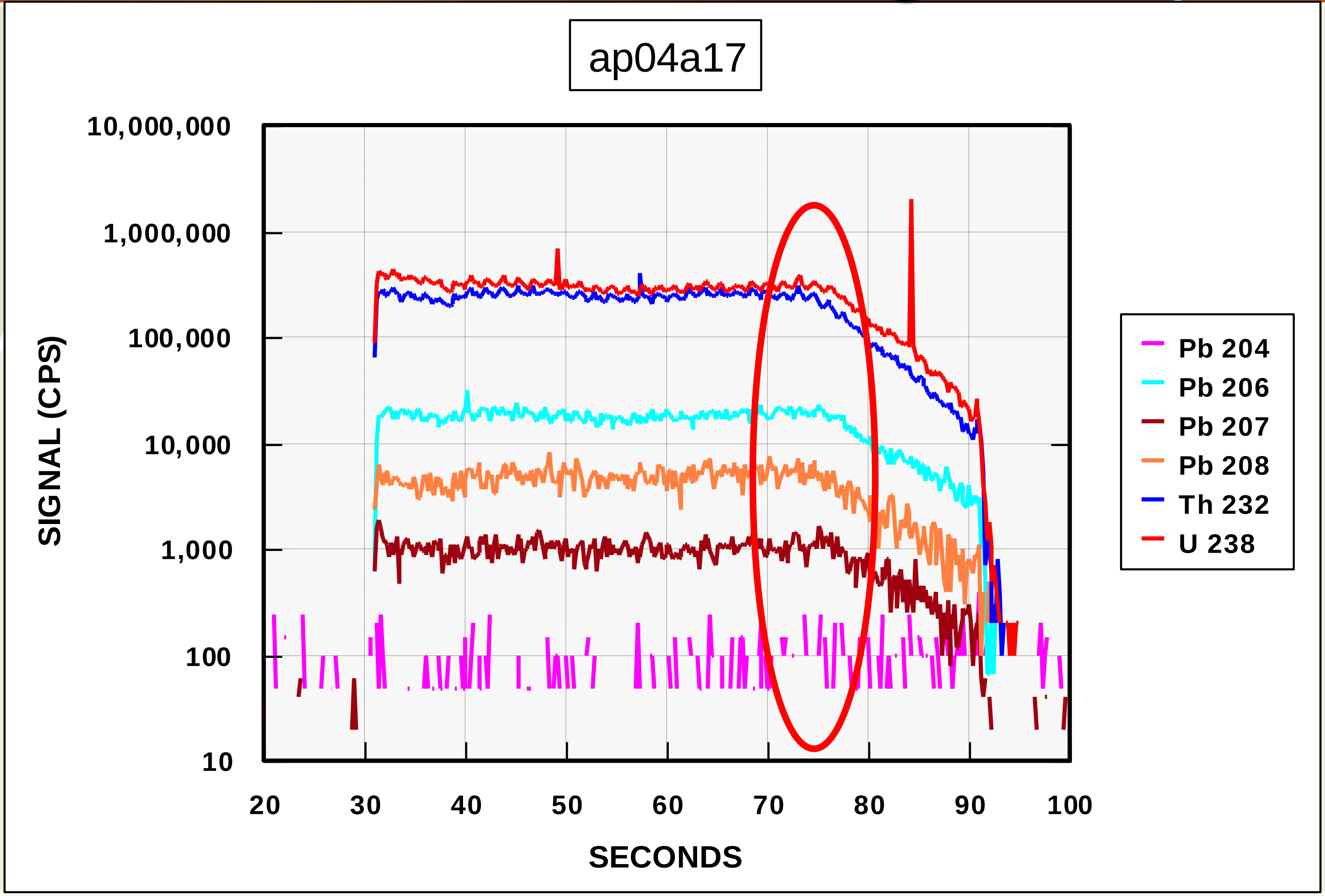
Zircon Z9910 ID-TIMS data



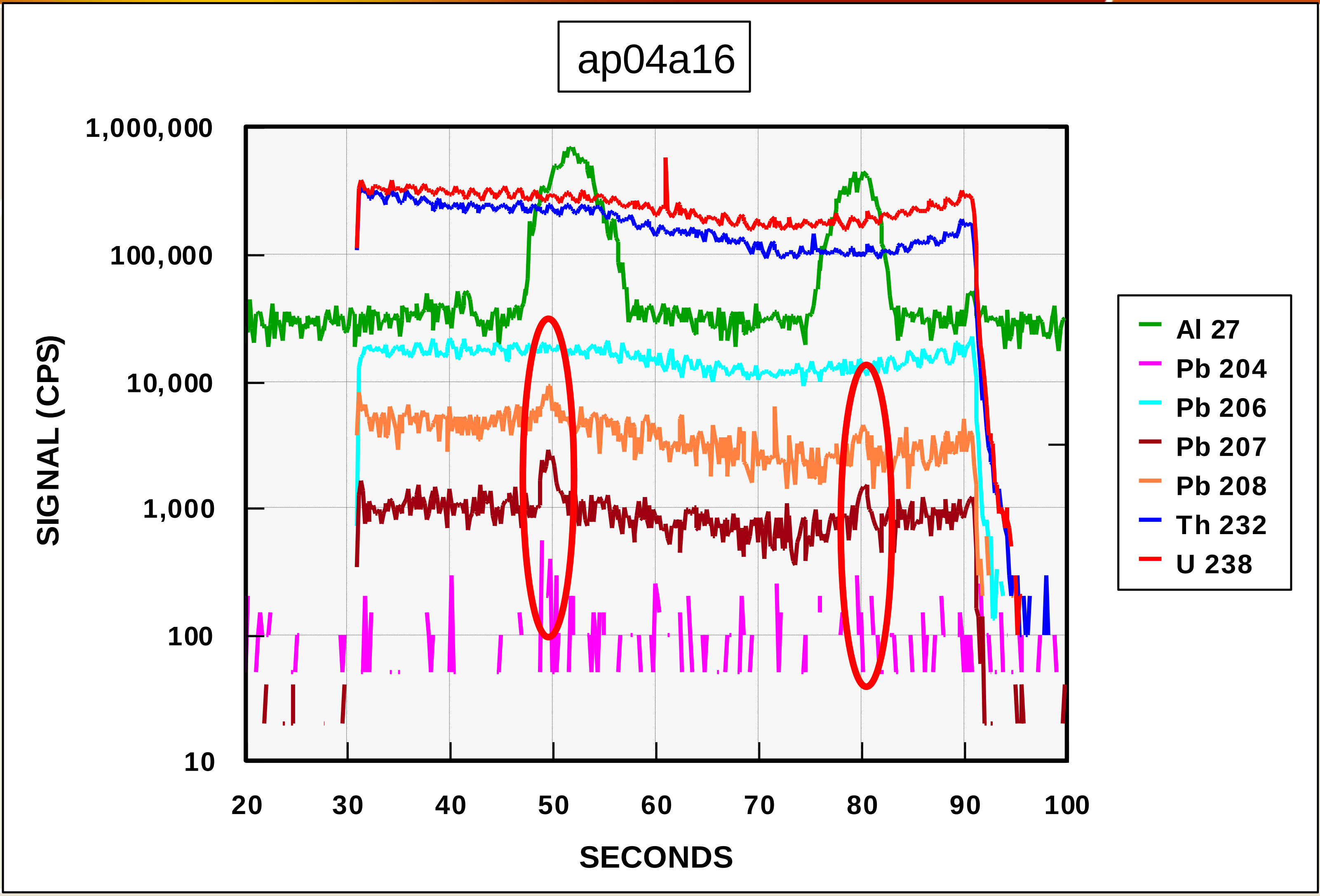
Zircon 91500



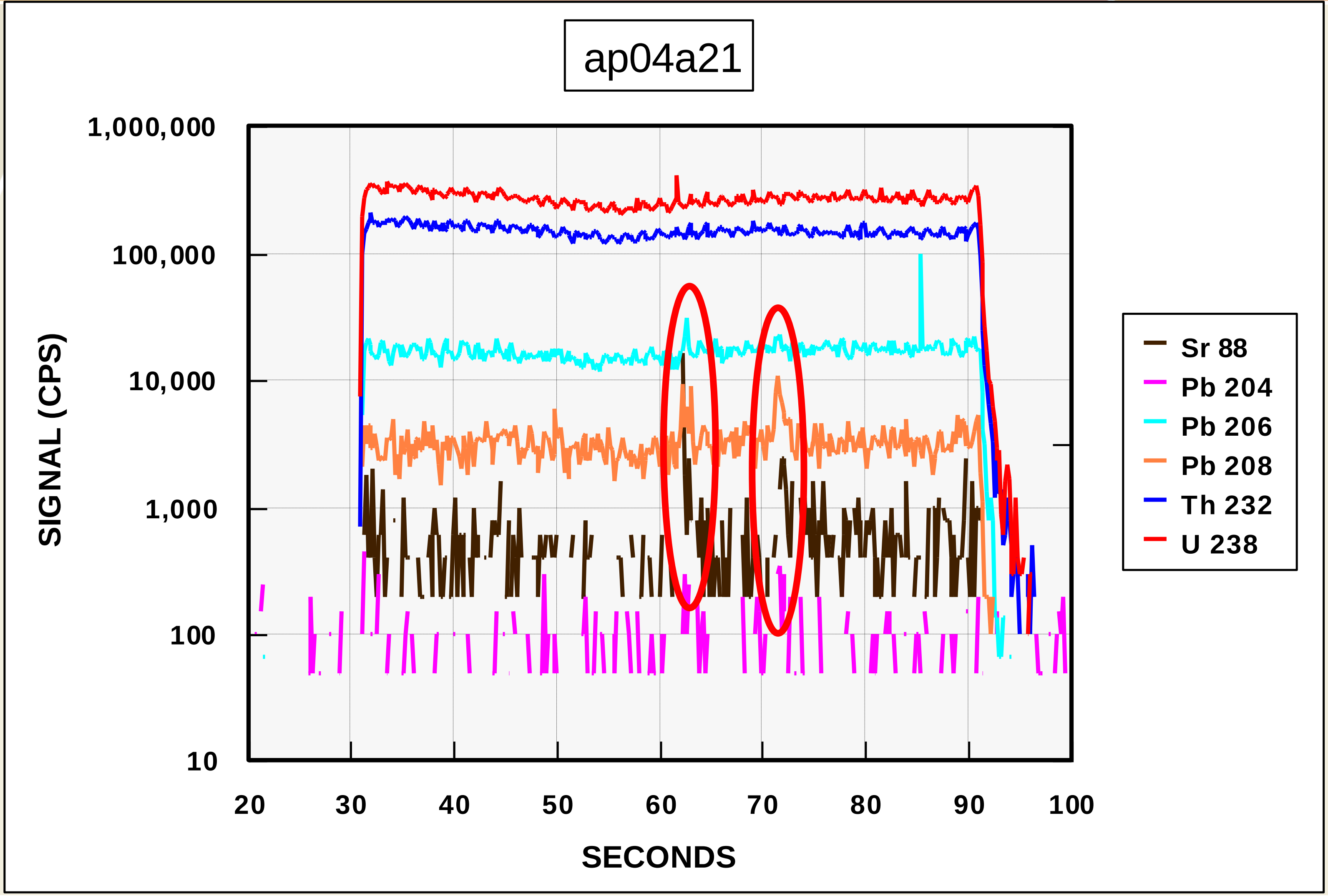
Zircon Z9910
Drill through



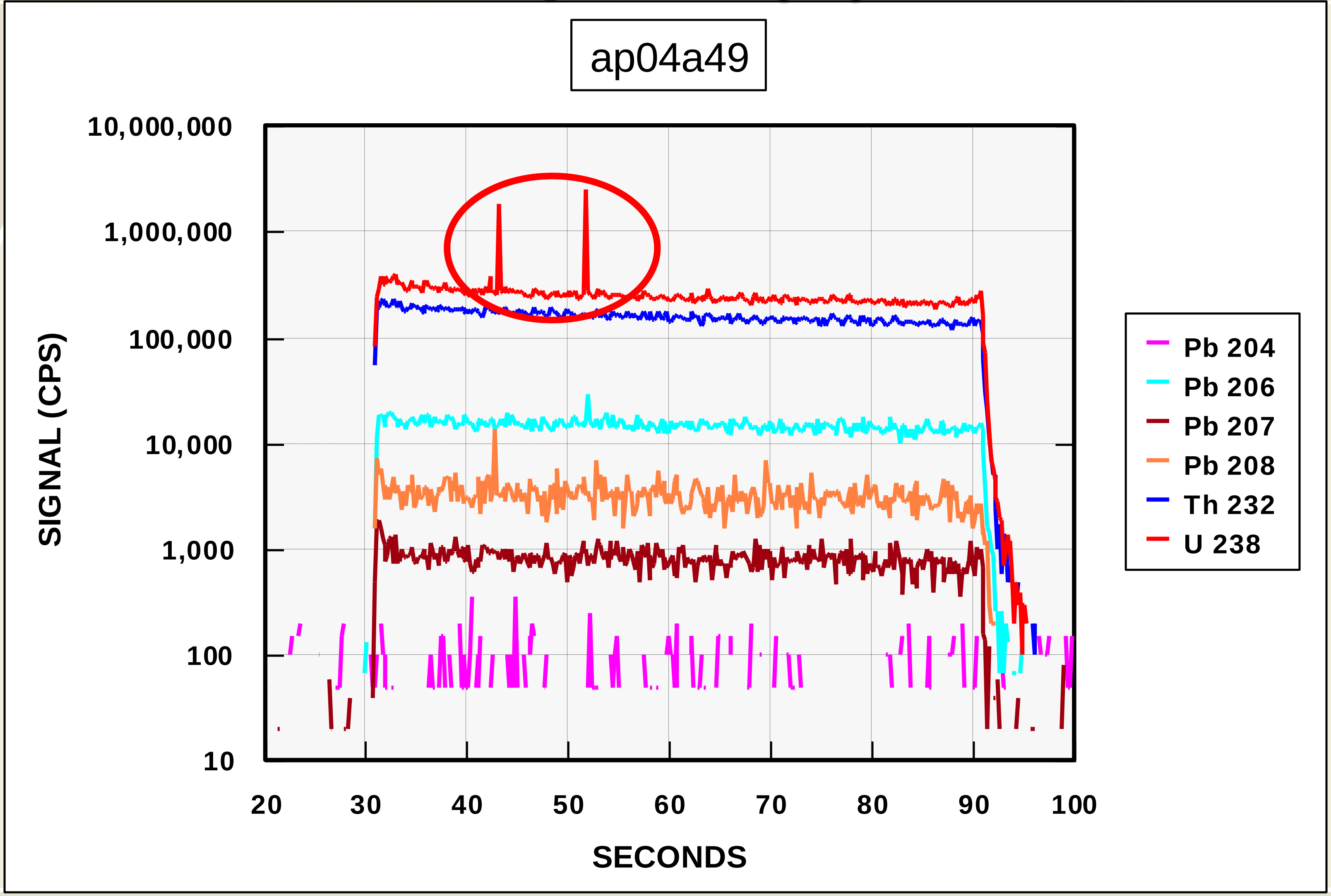
Zircon Z9910 Common Pb



Zircon Z9910
Common Pb



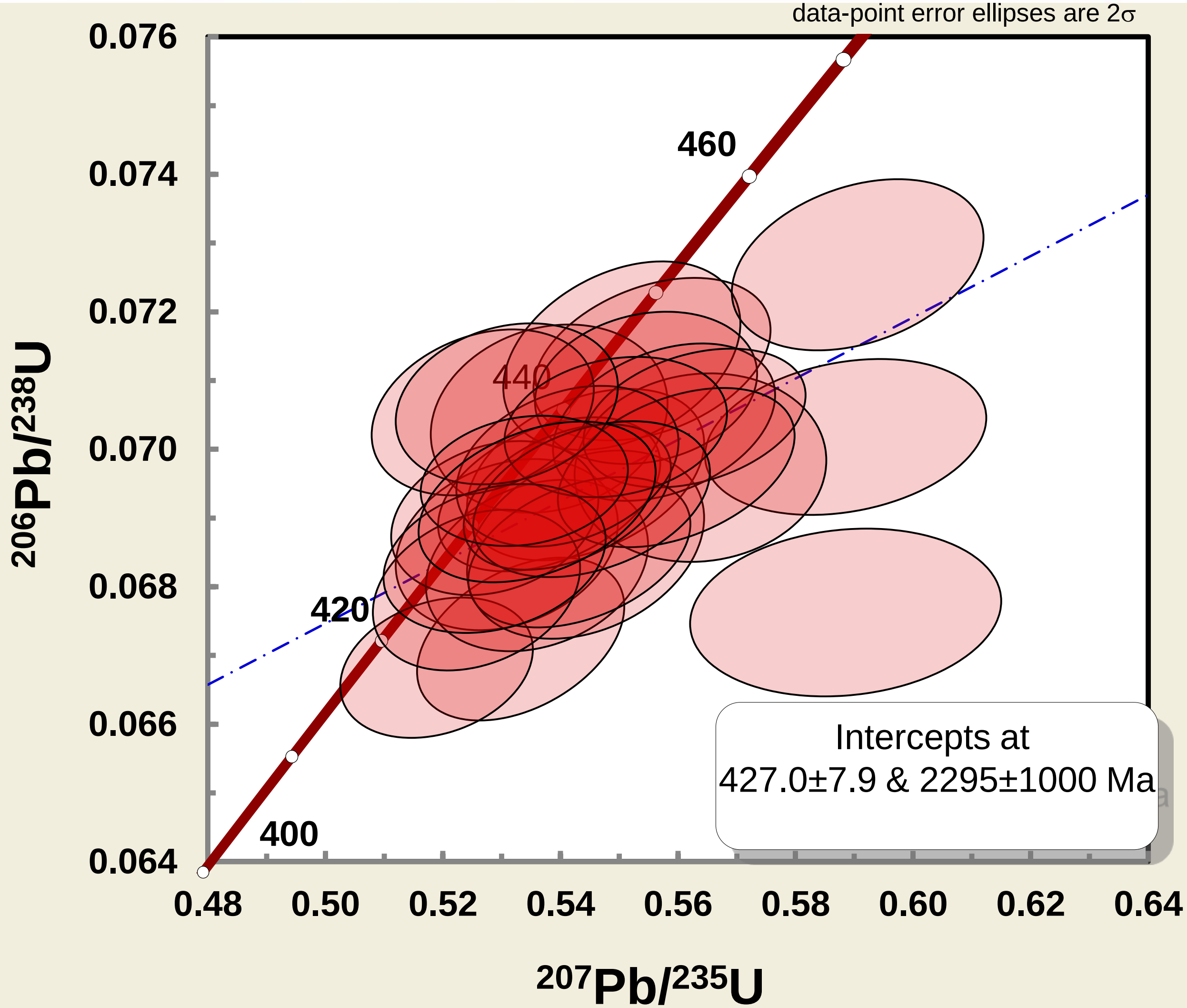
Zircon Z9910
Spikes (U)



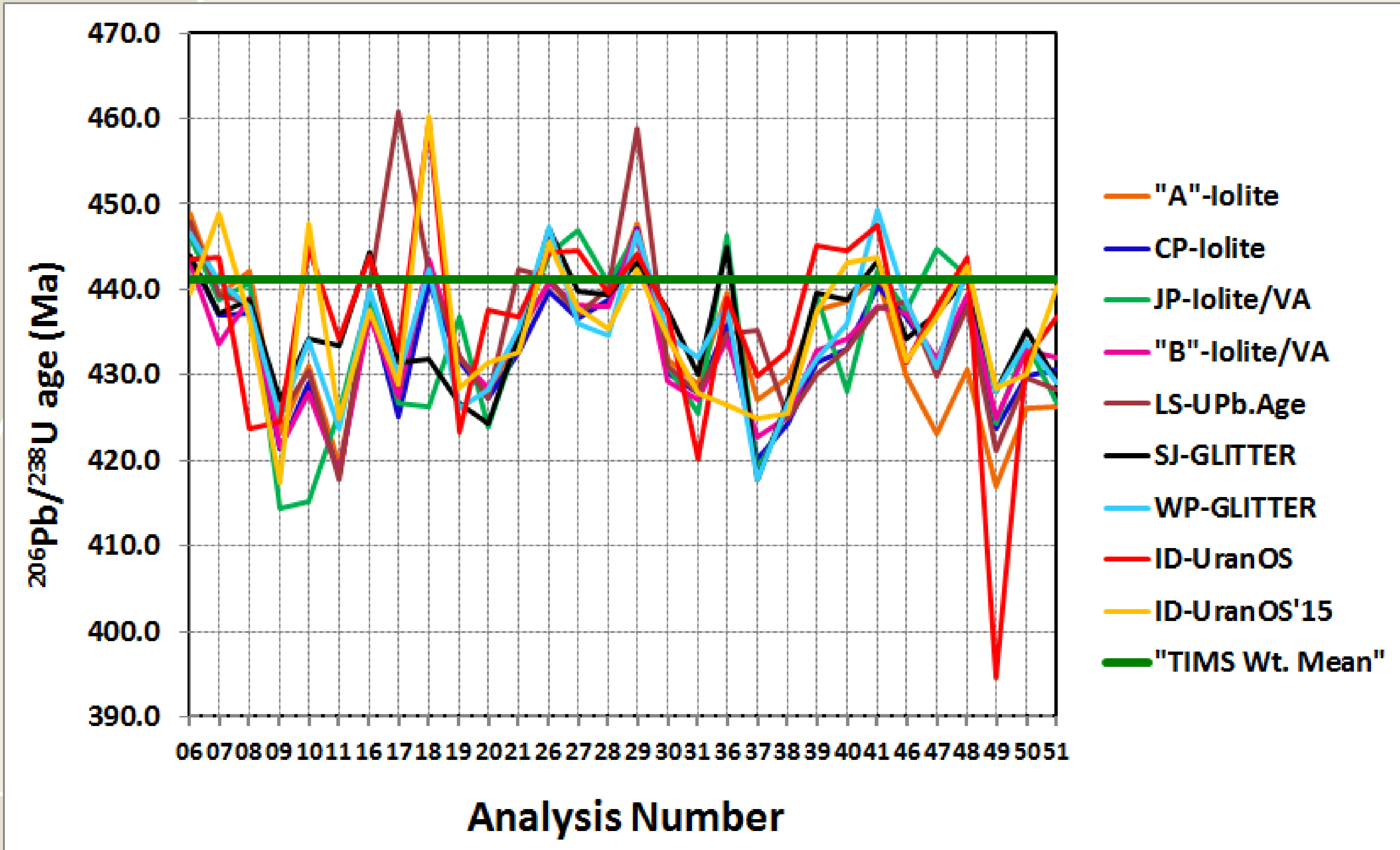
Software Packages Evaluated

Software	Operator	ID.	Version and comments
Iolite	"A" C. Paton	"A" CP	v. 2.3 v. 2.5, UPb_Geochronology3
Iolite/VizualAge	J. Petrus "B"	JP "B"	VA DRS v. 2013.02, Iolite v. 2.5, Exponential fractionation model VA DRS v. 2013.02, Iolite v. 2.5, Double exponential fractionation model, no Pbc
UPb.Age	L. Scolari	LS	v. 300413
GLITTER	W. Powell S. Jackson	WP SJ	v. 4.4.4 v. 4.4.2, spikes filtered
UranOS	I. Dunkl I. Dunkl	ID ID'15	v. 2.01 v. 2.06
UPb Redux	N. McLean	NM	Not included

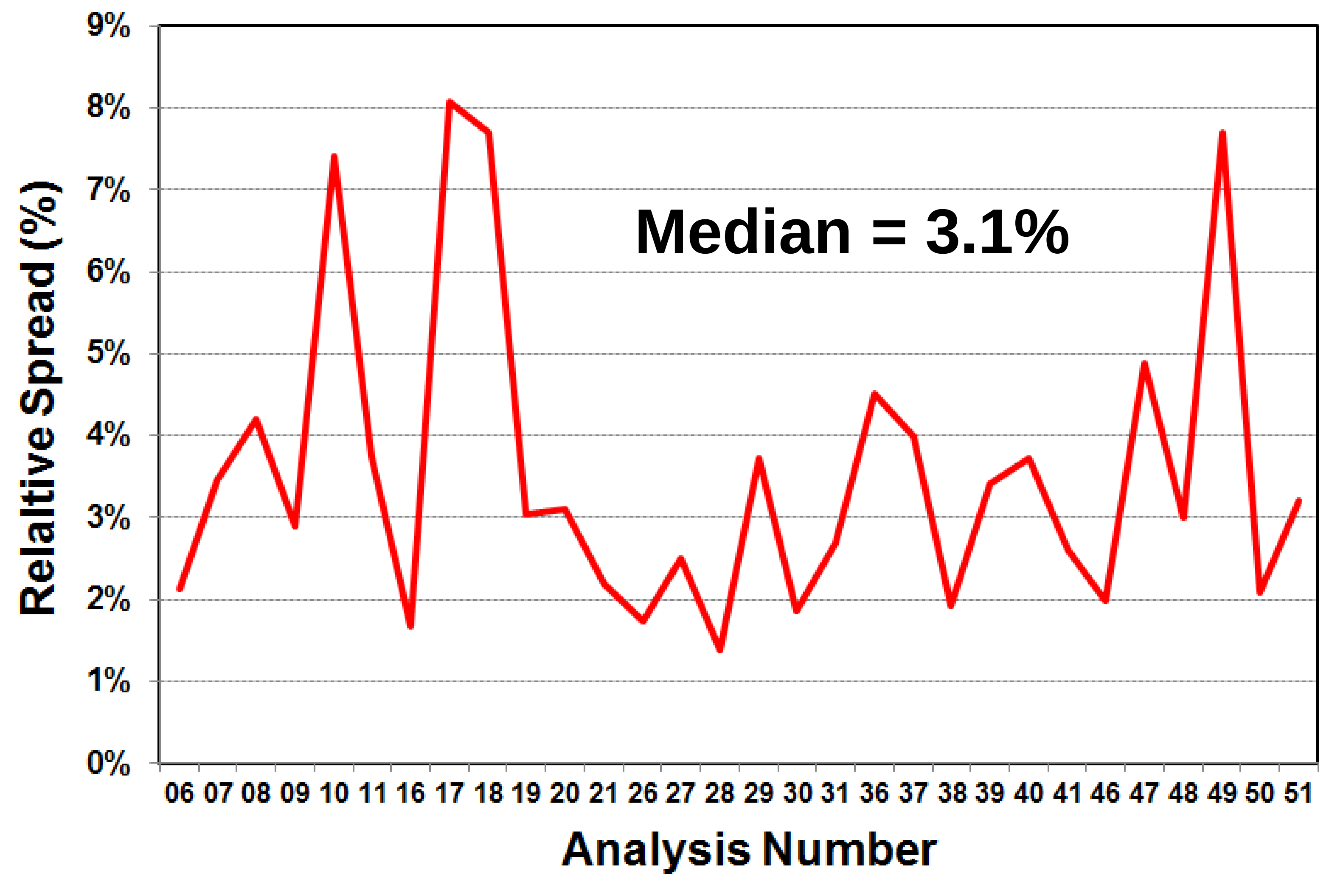
Zircon Z9910
Whole signal integrated



Zircon Z9910
$^{206}Pb/^{238}U$ Ages

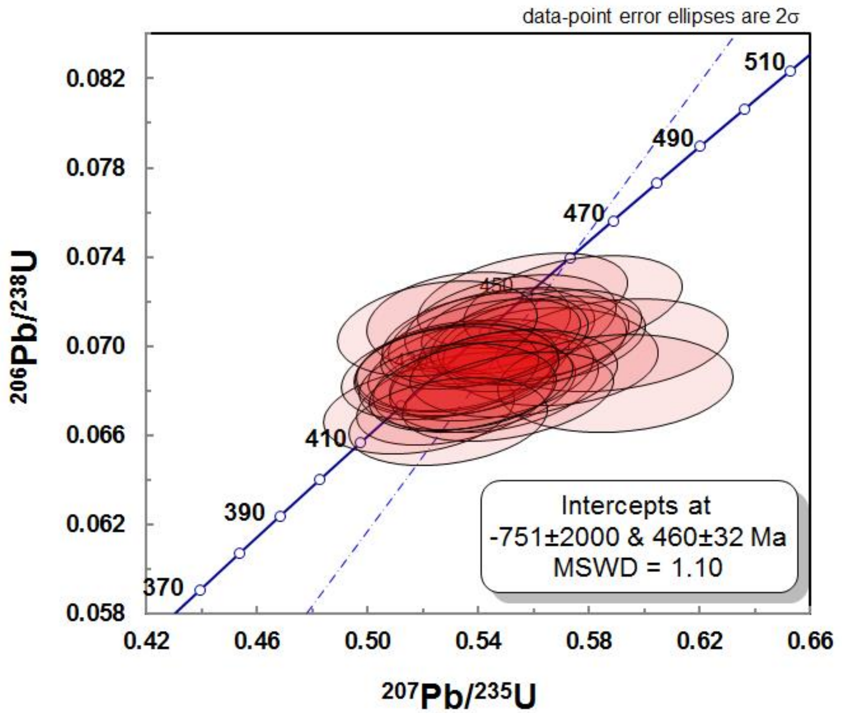


$^{206}Pb/^{238}U$ Age
Relative Spread in Data (Max-Min)

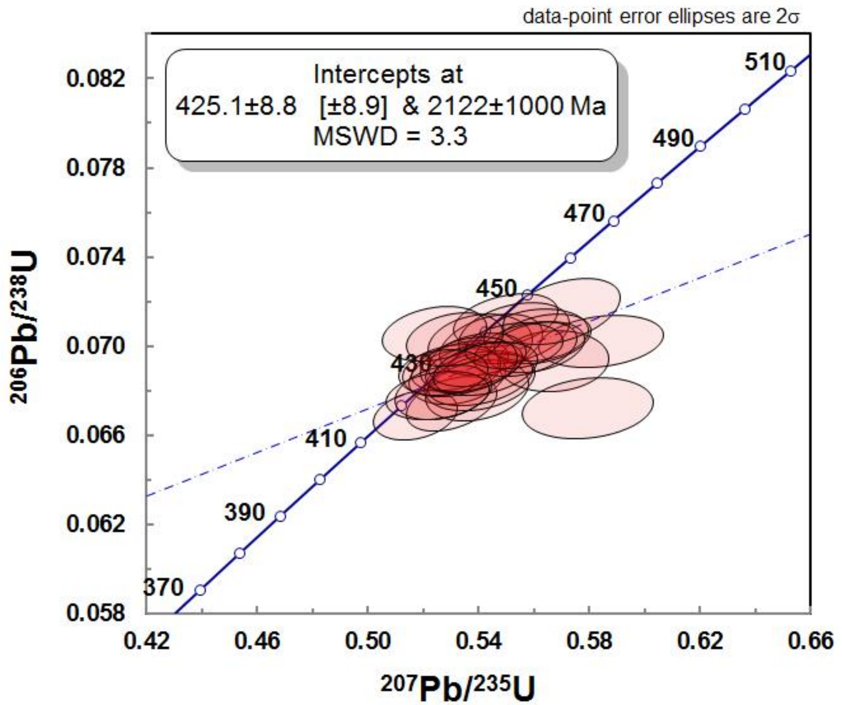


Iolite Concordia

"A"

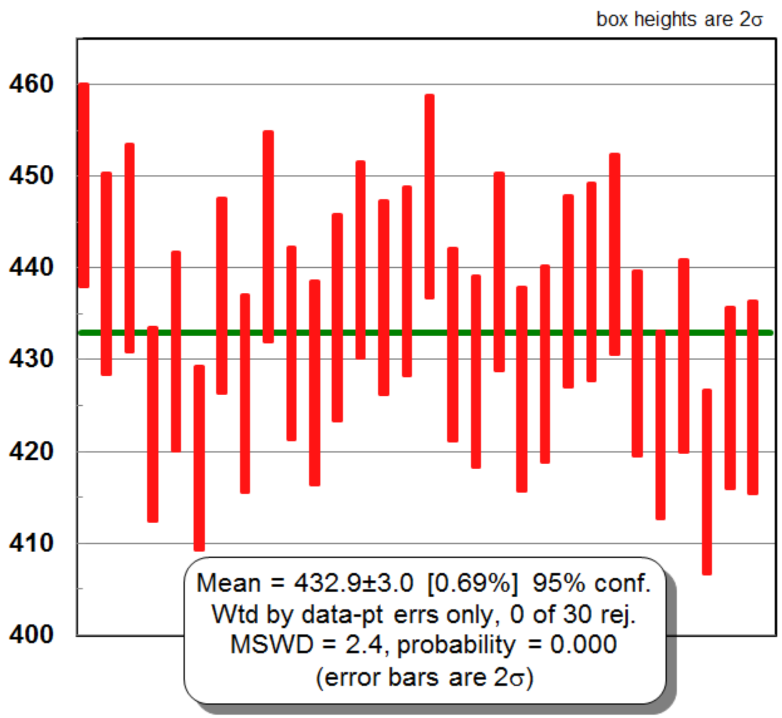


CP

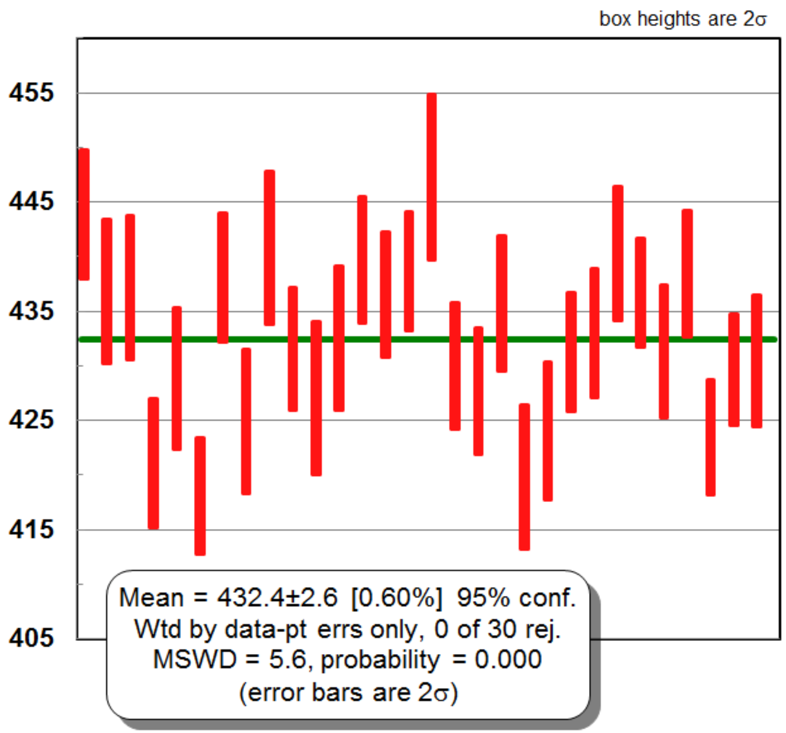


Iolite
Weighted Mean $^{206}Pb/^{238}U$ Age

"A"

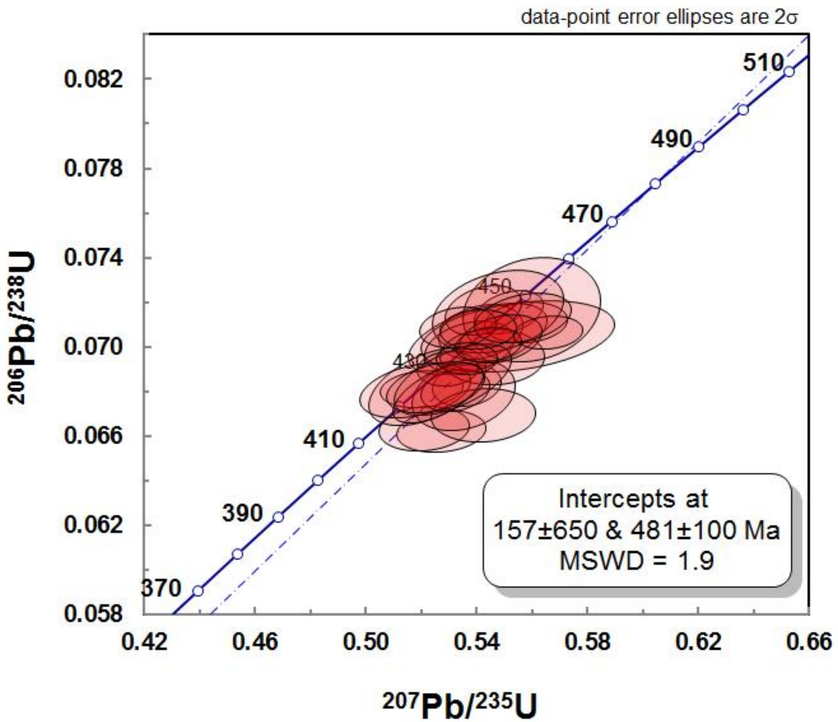


CP

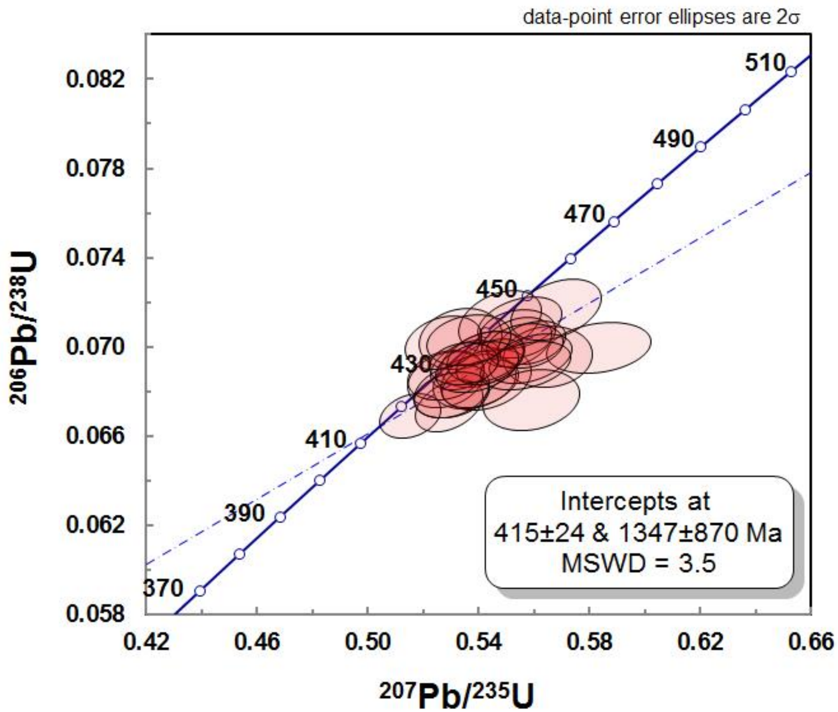


Iolite/VizualAge Concordia

JP

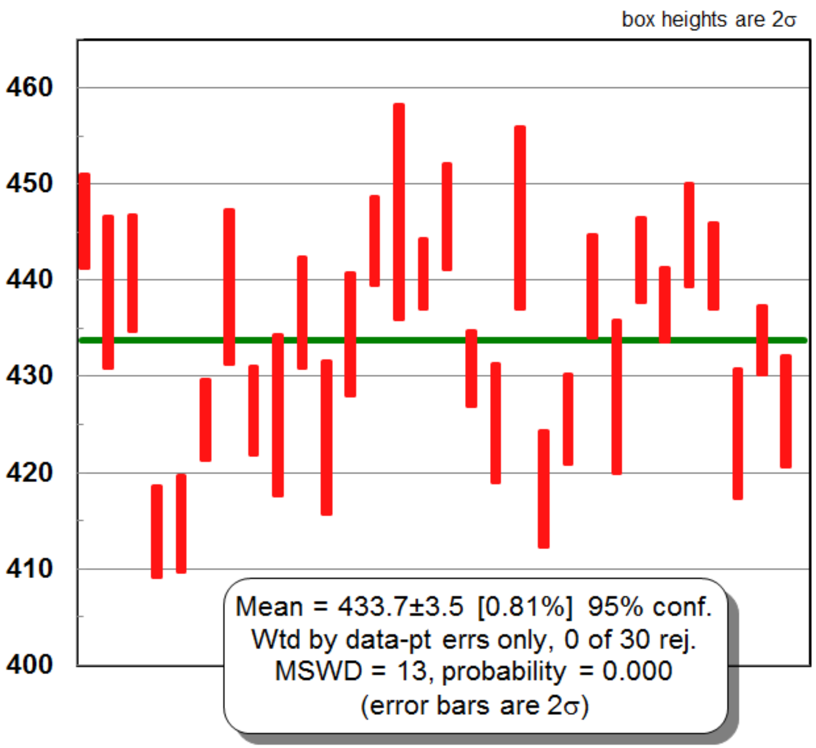


"B"

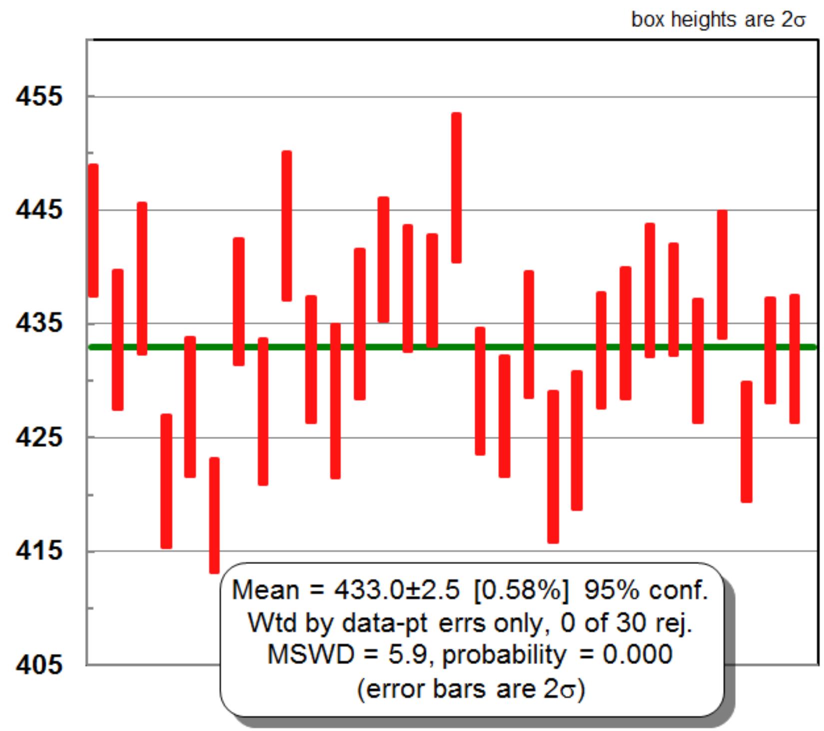


Iolite/VizualAge
Weighted Mean $^{206}Pb/^{238}U$ Age

JP

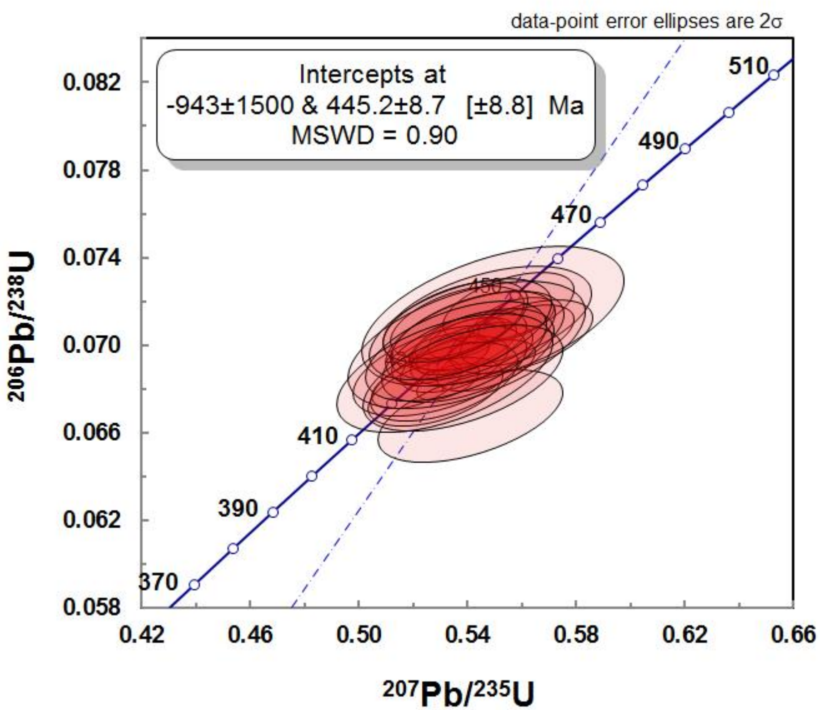


"B"

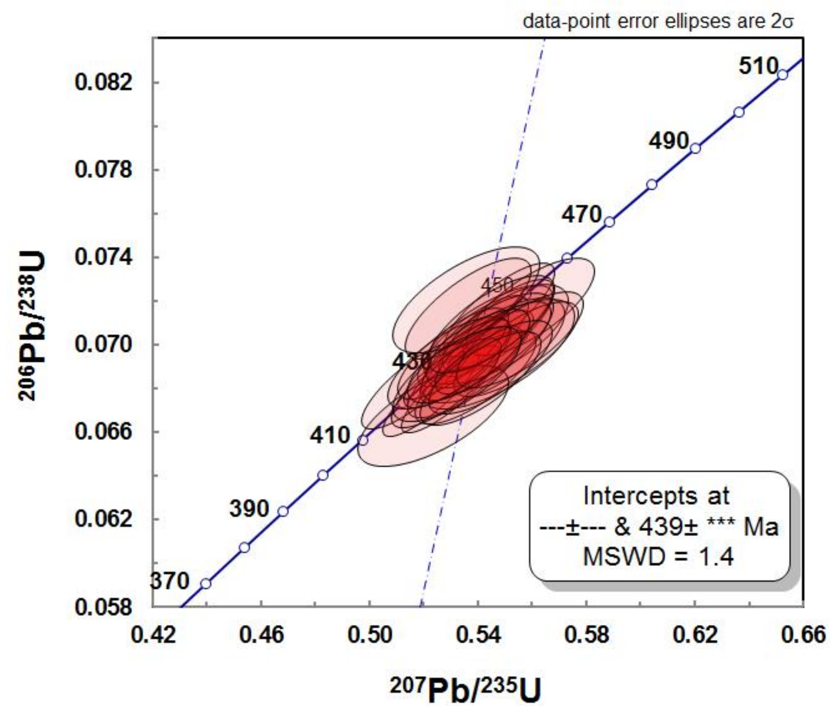


GLITTER
Concordia

SJ

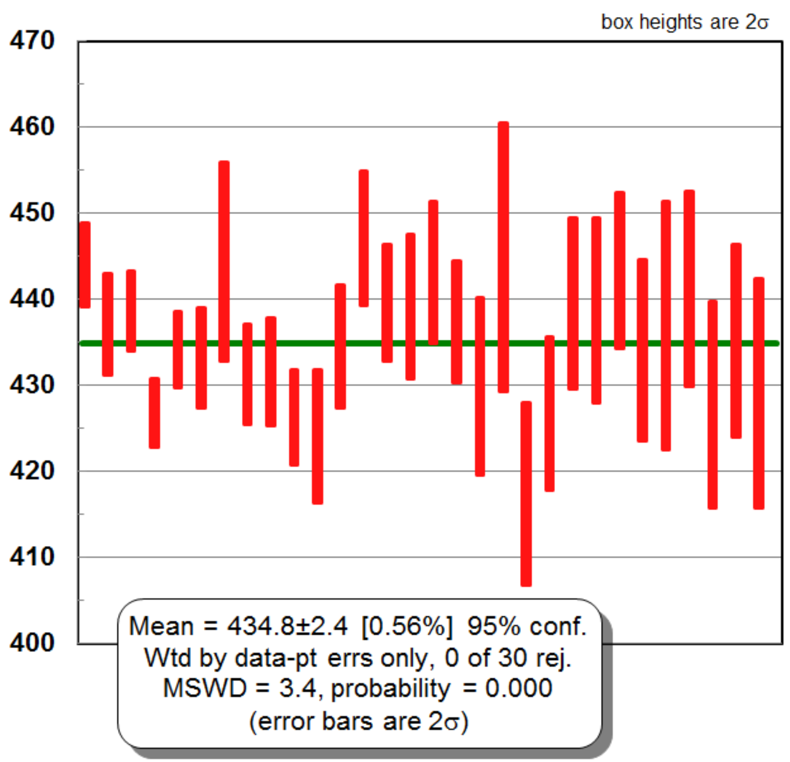


WP

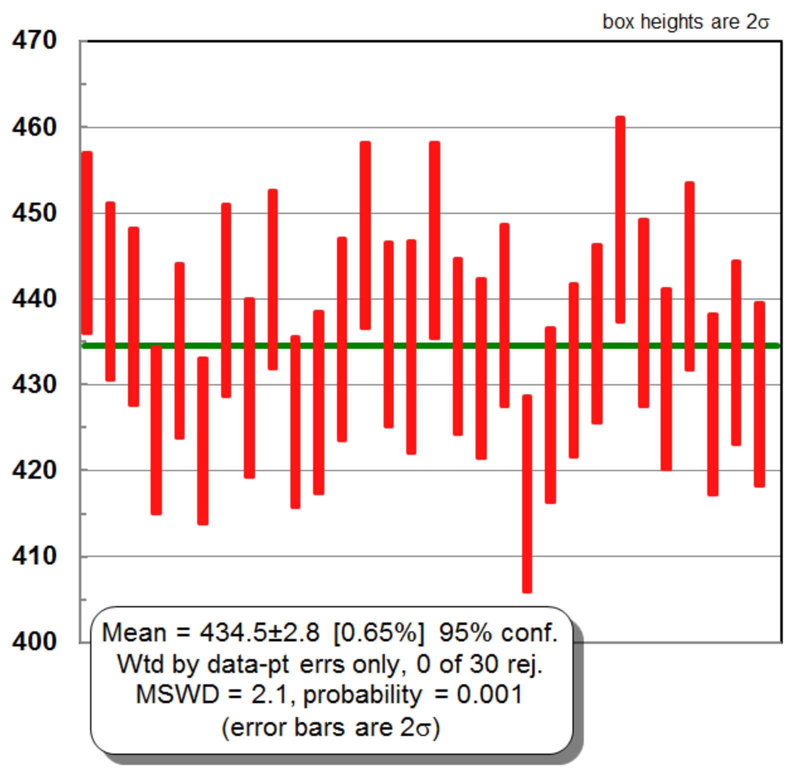


GLITTER
Weighted Mean $^{206}Pb/^{238}U$ Age

SJ

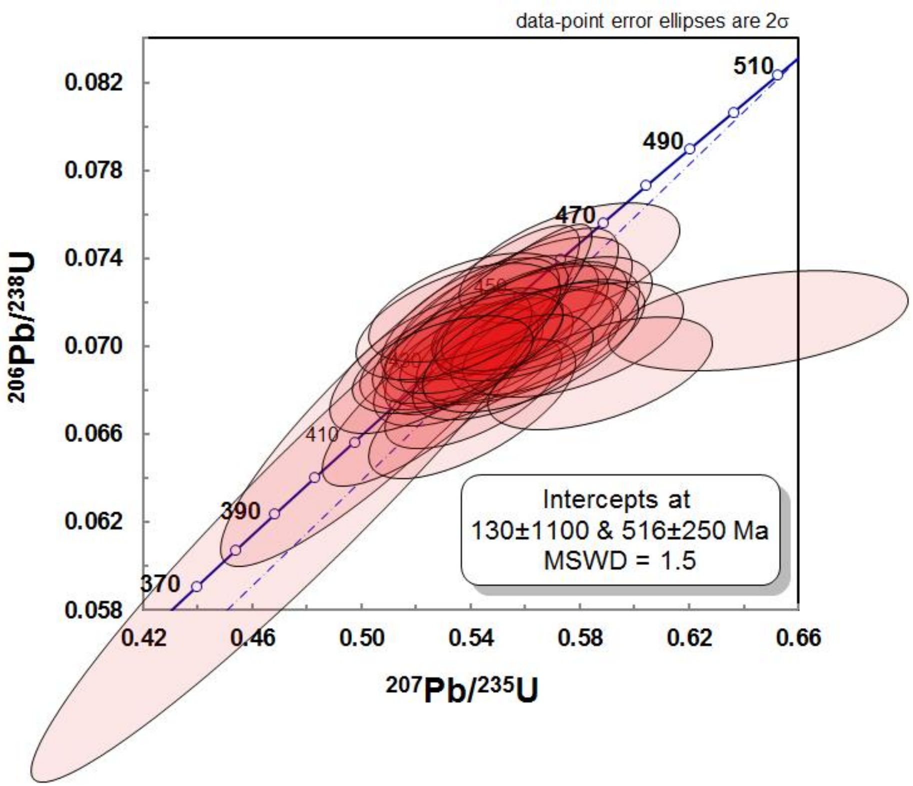


WP

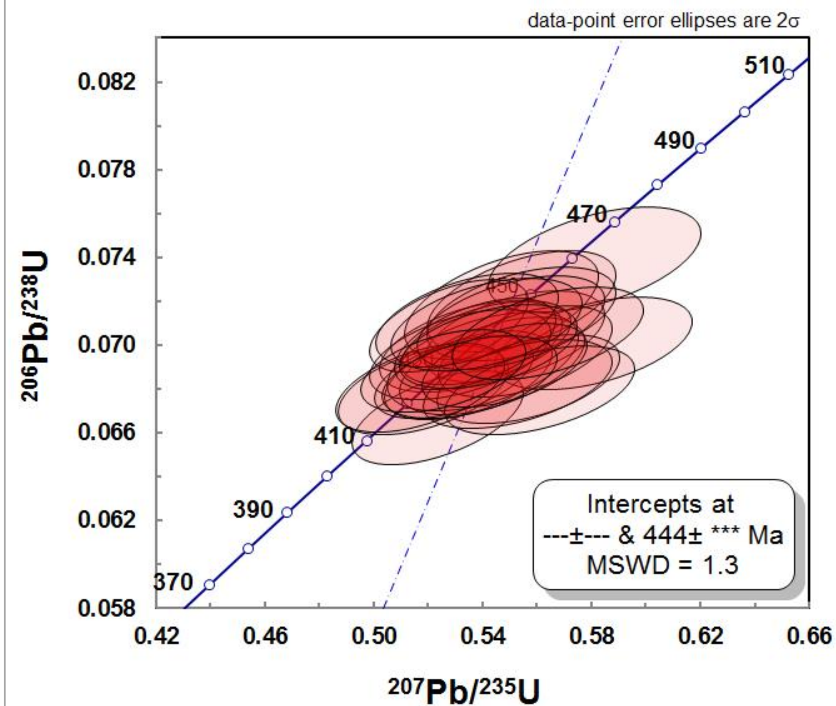


UranOS Concordia

ID

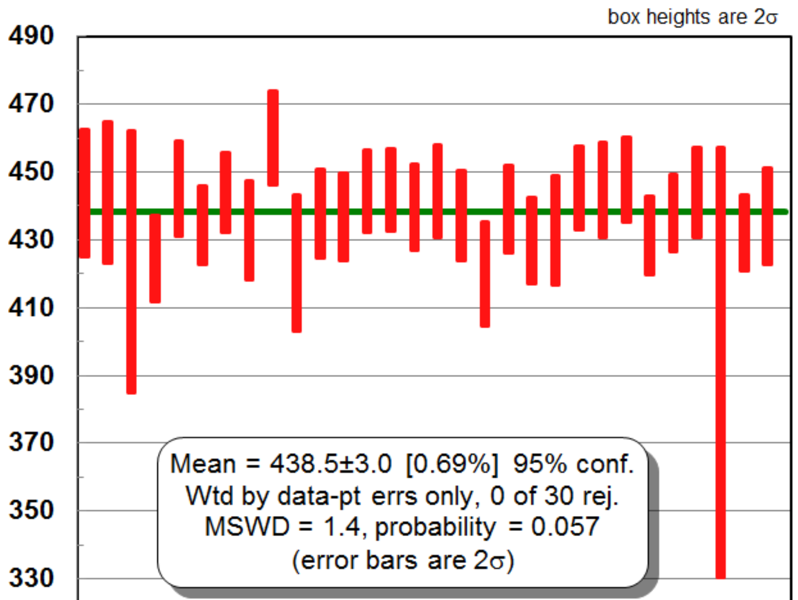


ID'15

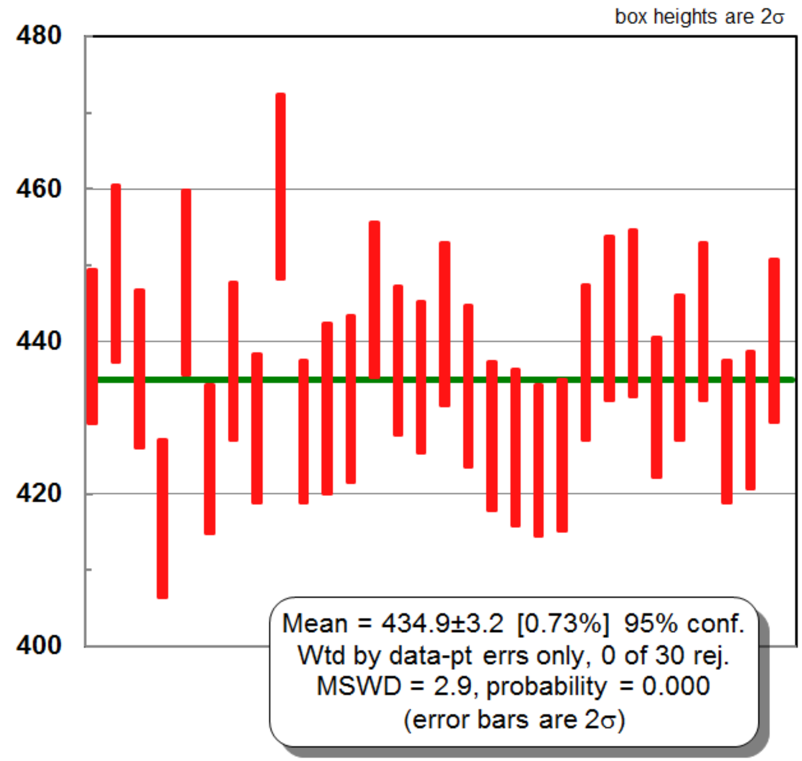


UranOS
Wt. Mean $^{206}Pb/^{238}U$ Age

ID



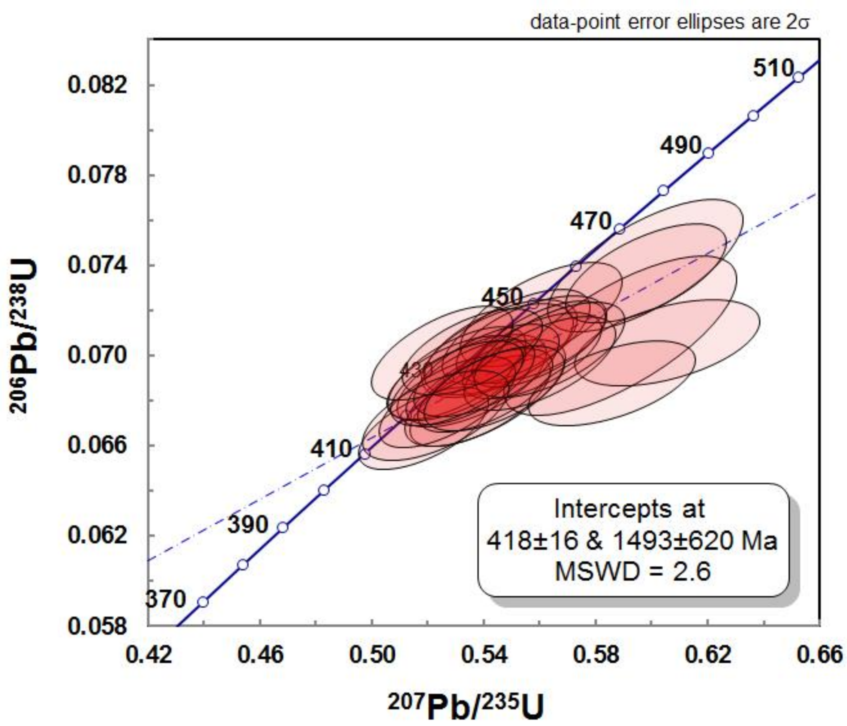
ID'15



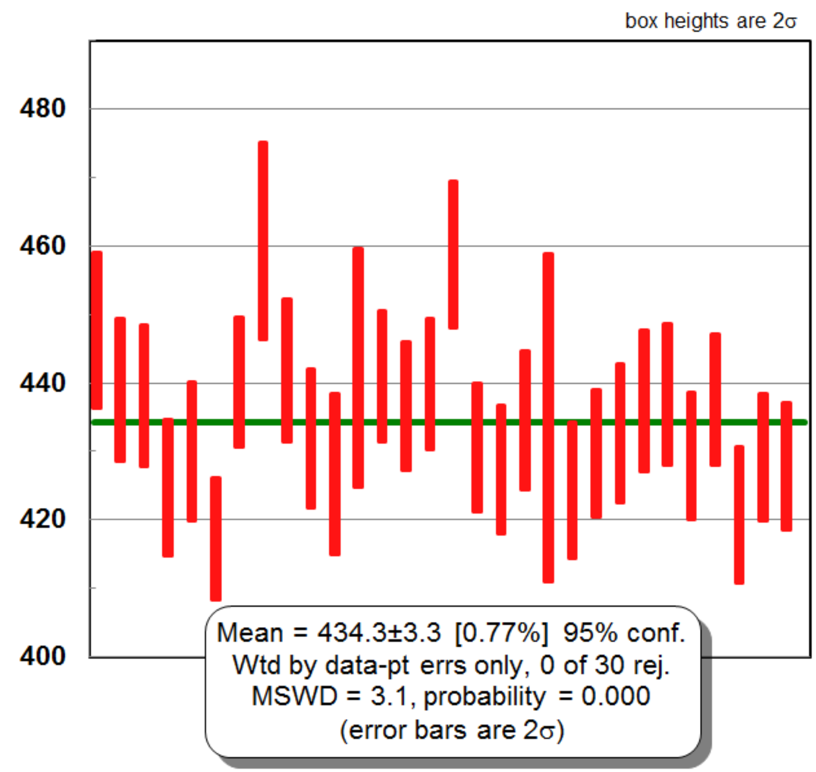
UPb.Age

Concordia and Weighted Mean $^{206}Pb/^{238}U$ Age

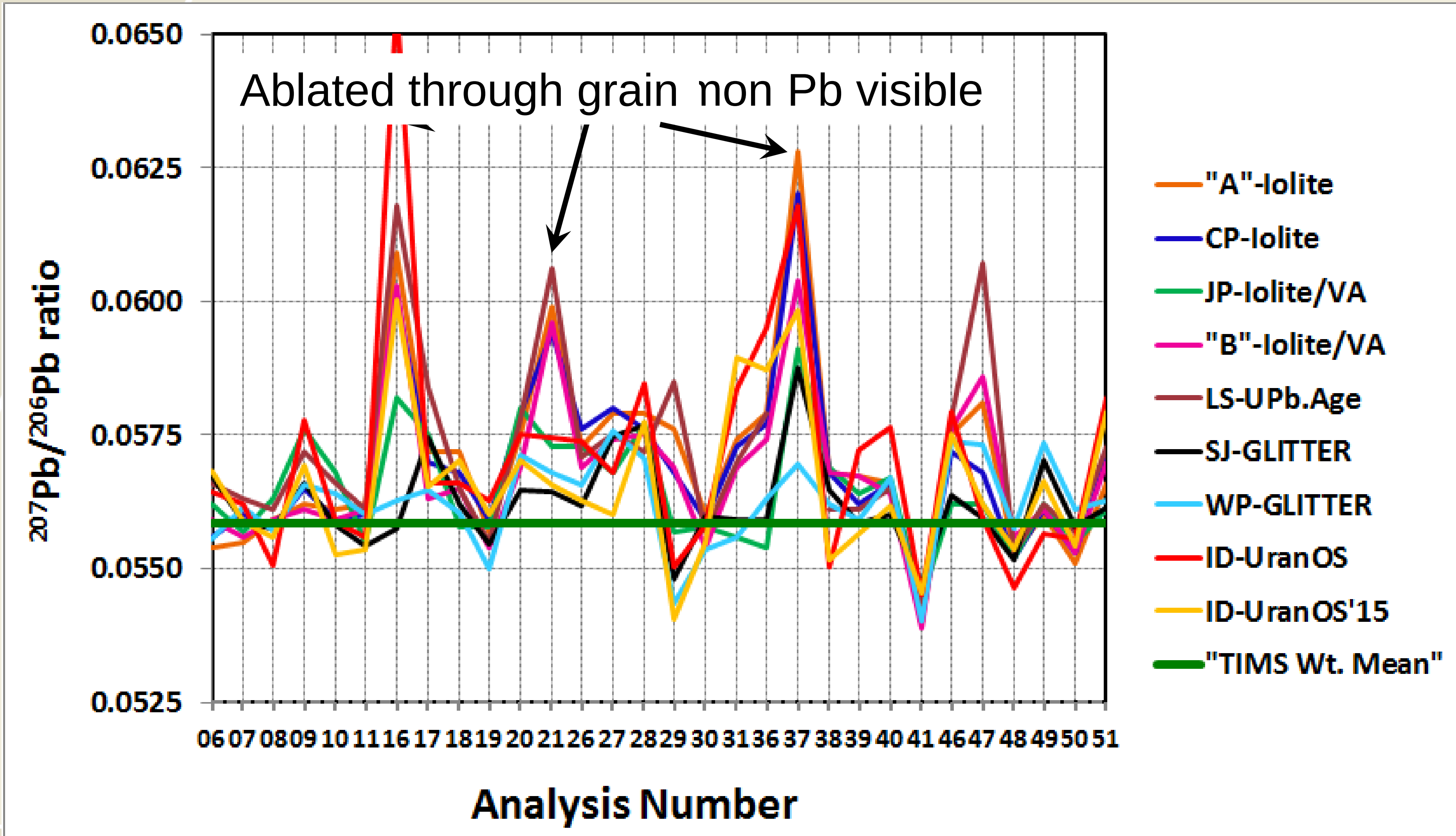
LS



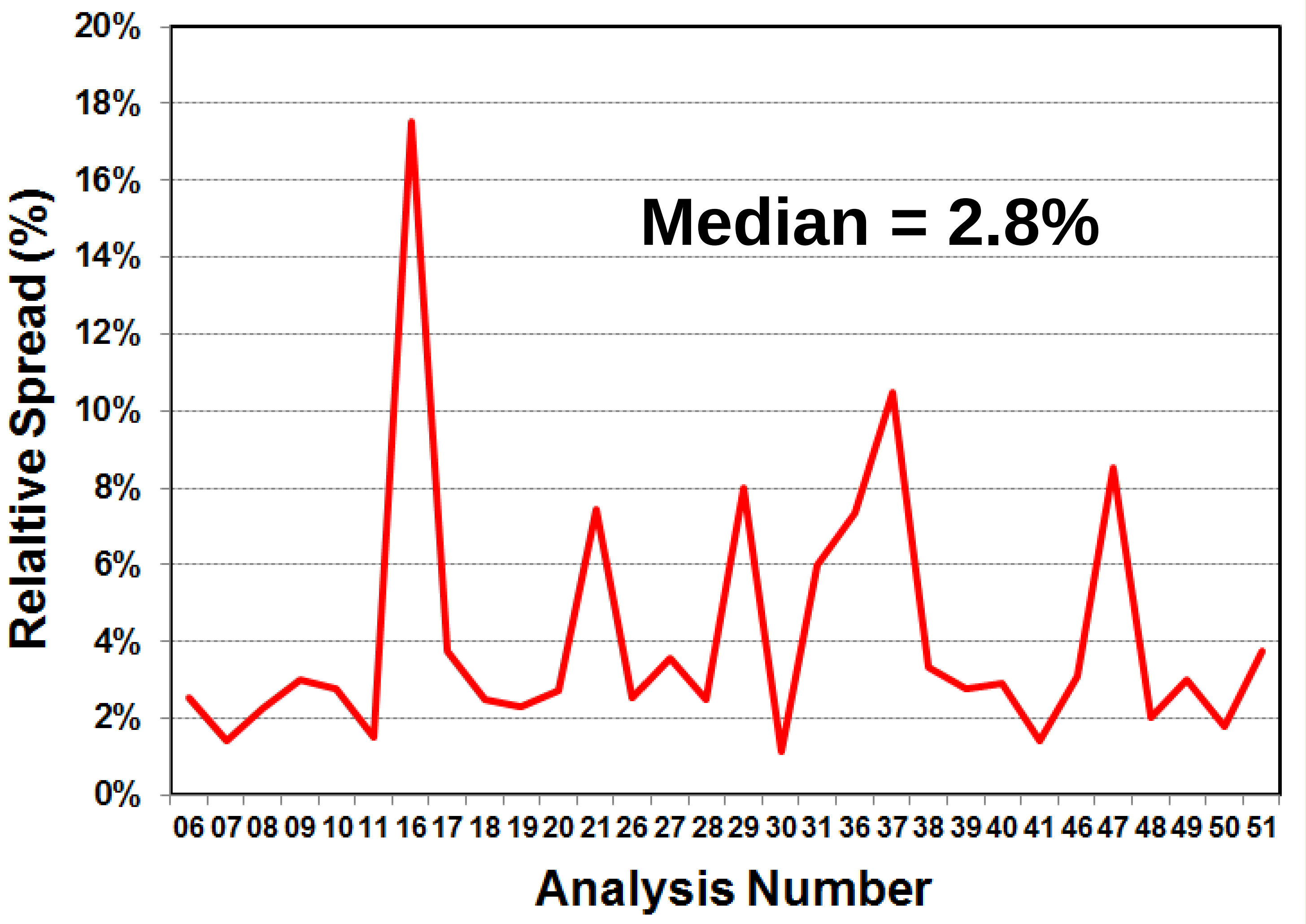
LS



Zircon Z9910
$^{207}Pb/^{206}Pb$ Ratios



$^{207}Pb/^{206}Pb$ Ratio
Relative Spread in Data (Max-Min)



Summary

ID	Wt. Mean 206/238 Age				Wt. Mean 207/206 Ratio			
	age (Ma)	95% conf	MSWD	Rel. Diff.	ratio	95% conf	MSWD	Rel. Diff.
"A"-Iolite	432.9	3.0	2.4	1.9%	0.05689	1.05%	1.6	-1.9%
CP-Iolite	432.4	2.6	5.6	2.0%	0.05675	0.86%	3.3	-1.6%
JP-Iolite/VA	433.7	3.5	13	1.7%	0.05632	0.60%	1.9	-0.9%
"B"-Iolite/VA	433.0	2.5	5.9	1.8%	0.05659	0.81%	4.4	-1.3%
SJ-GLITTER	434.8	2.4	3.4	1.4%	0.05620	0.62%	0.60	-0.6%
WP-GLITTER	434.5	2.8	2.1	1.5%	0.05619	0.57%	0.79	-0.6%
ID-UranOS	438.5	3.0	1.4	0.6%	0.05680	1.16%	2.1	-1.7%
ID'15-UranOS	434.9	3.2	2.9	1.4%	0.05646	0.92%	1.4	-1.1%
LS-UPb.Age	434.3	3.3	3.1	1.6%	0.05687	0.95%	2.8	-1.8%
Max	438.5	3.5	13.0	2.0%	0.05689	1.16%	4.4	-0.6%
Min	432.4	2.4	1.4	0.6%	0.05619	0.57%	0.6	-1.9%
Rel. Diff.	1.4%				1.3%			

Conclusions

- Processing of LA-ICP-MS U/Pb data induces significant variations in the results. In this study, typically:
  - Ca. 3.1% on an individual $^{206}Pb/^{238}U$ age, 2.8% on an individual $^{207}Pb/^{206}Pb$ ratio
  - Up to 1.4% on the weighted mean $^{206}Pb/^{238}U$ age, 1.3% on the weighted mean $^{207}Pb/^{206}Pb$ ratio
  - Encouragingly, excluding 1 result, the spread of weighted mean $^{206}Pb/^{238}U$ ages is only 0.6% (± 0.3%)
  - However, the excluded result is the only one that agrees with the ID-TIMS age (within 95% confidence interval)
- All weighted mean $^{206}Pb/^{238}U$ ages are young (0.6-2.0%)
  - Various approaches to correct Pb/U fractionation operate equally well, but are not perfect (precise but not accurate)
- Results are both software and operator dependent

Conclusions

- MSWD's for the weighted mean $^{206}Pb/^{238}U$ ages are all >1, mostly >2, indicating excess scatter (observed scatter exceeds that predicted by the quoted uncertainties):
  - variable Pb/U fractionation
  - single channel spikes, especially U
  - common Pb
- MSWD's for $^{207}Pb/^{206}Pb$ are >1, except one package (both users)
  - Low MSWD's seem to reflect more effective avoidance of common Pb through judicious signal interval selection
- No reported data were common Pb-corrected (?) despite significant evidence of its presence
- The differences in reported ages and uncertainties are sufficient to cause significant differences in interpreted age when using unconstrained regressions

Recommendations

- Need to explore new approaches to mitigate/correct Pb/U fractionation
  - Annealing?
  - New software corrections
- Need to instigate and more widely apply common-Pb correction

AND, as ever,

- Judicious (painstaking) selection of integration intervals to avoid common Pb (Al, Sr, Ba), zones of Pb loss, and other artefacts
- Still need to instigate/apply more robust error propagation (see Horstwood et al., submitted)