

## Mass spectrometry

## Performance of Neoma MS/MS MC-ICP-MS for analysis of radiogenic isotopes



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### Keywords

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### Goal

To show performance of Thermo Scientific™ Neoma™ MS/MS MC-ICP-MS for analysis of non-traditional radiogenic isotopes.

### Introduction

Radiogenic isotopes are produced by the decay of radioactive nuclei and are versatile tools in Earth sciences. In geochronology, they are used to determine the timescales of geological processes ranging from ages of individual minerals to the timescales of large-scale chemical differentiation of asteroids and terrestrial planets. As tracers of geological processes, radiogenic isotopes provide information on rates and pathways of geological processes, including the compositional evolution of the Earth and other planetary bodies, processes of planetary differentiation, as well as identifying the origin of Earth's water.

Amongst the radiogenic isotopes, hafnium ( $^{176}\text{Hf}$ ), lead ( $^{206}\text{Pb}$ ,  $^{207}\text{Pb}$ ,  $^{208}\text{Pb}$ ), neodymium ( $^{142}\text{Nd}$ ,  $^{143}\text{Nd}$ ), and strontium ( $^{87}\text{Sr}$ ), are the most widely used within geoscience applications. The isotopic ratios of these elements can be measured at high precision using the Neoma MC-ICP-MS. For multi-user laboratories that require MS/MS functionality for other applications, it is important to be able to measure these core isotope systems with the same degree of accuracy and precision as with the Neoma MC-ICP-MS. Here we demonstrate the performance of the Thermo Scientific™ Neoma™ MS/MS MC-ICP-MS for hafnium, lead, neodymium and strontium across 9 instruments.

## Method

Nine Neoma MS/MS MC-ICP-MS instruments underwent performance tests for accuracy and precision within the Bremen factory. In all experiments (Table 1), the pre-filter slit position was set to 100%, i.e. full ion transmission, and there was no gas within the collision/reaction cell. Samples were analyzed in wet plasma for a total of 10 minutes each. The cup configurations are listed in Table 2. Interference corrections and exponential mass bias corrections were applied (Table 1). Note that samples were not standard-sample bracketed.

## Results and Interpretation

### Sensitivity

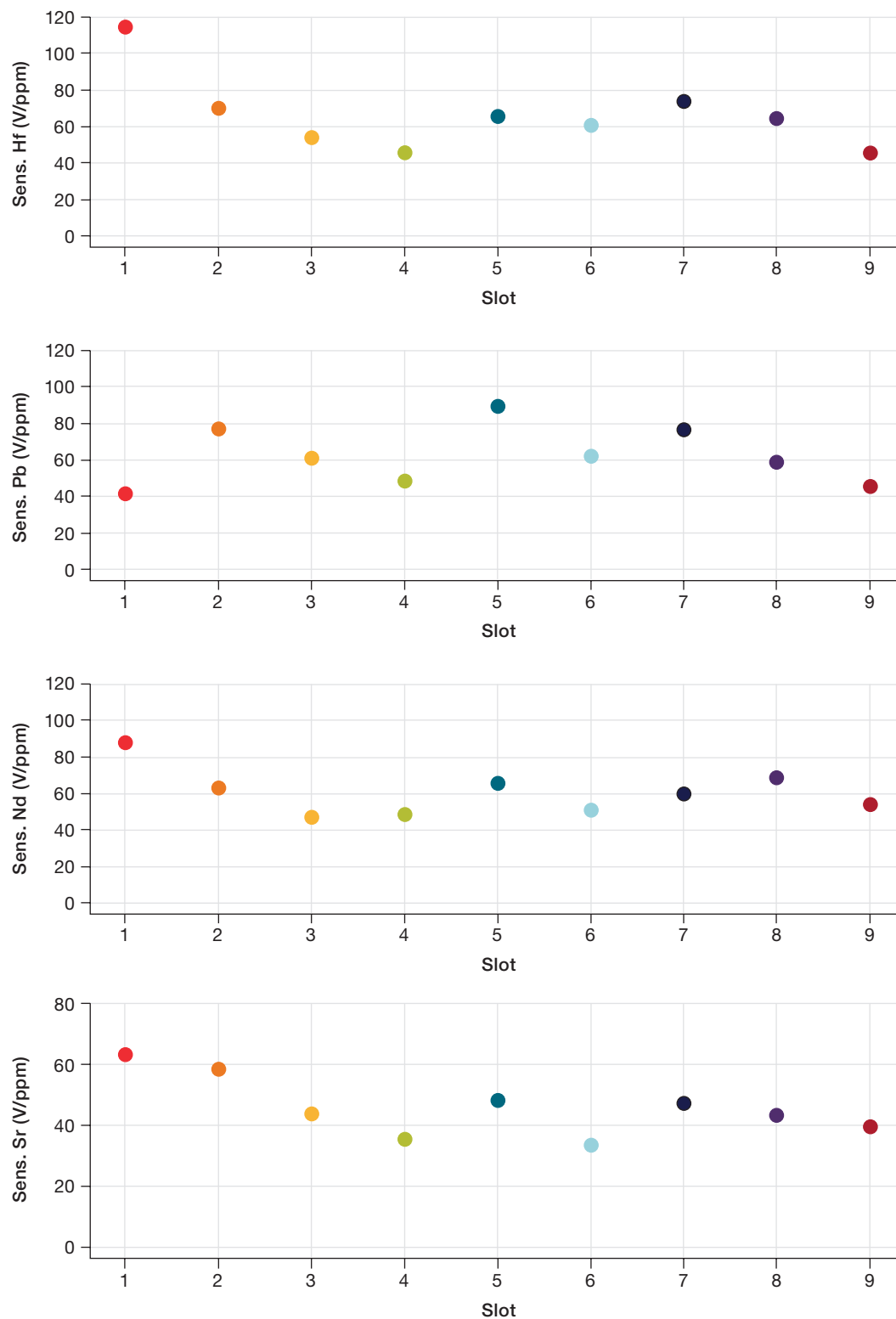
Sensitivity of the 9 systems is variable (Figure 1) as instruments were only crudely tuned to achieve sensitivities above the specification of 45 V/ppm, 50 V/ppm, 45 V/ppm and 40 V/ppm for Hf, Pb, Nd and Sr respectively. However, it can be seen that sensitivities of up to 110 V/ppm, 90 V/ppm, 90 V/ppm and 64 V/ppm for Hf, Pb, Nd and Sr respectively can be achieved. Note that these sensitivities are for wet plasma. In dry plasma, the specified sensitivities are over an order of magnitude greater.

Table 1. Experiment overview for analysis of hafnium, lead, neodymium and strontium

|                                   | Hafnium                                                    | Lead                                 | Neodymium                                                                        | Strontium                                                |
|-----------------------------------|------------------------------------------------------------|--------------------------------------|----------------------------------------------------------------------------------|----------------------------------------------------------|
| <b>Solution</b>                   | 100 ppb Hf<br>Merck™                                       | 100 ppb Pb<br>NIST® SRM® 981         | 100 ppb Nd<br>Merck™                                                             | 100 ppb Sr<br>NIST® SRM® 987                             |
| <b>Sample introduction system</b> | SIS spray chamber for Neoma MC-ICP-MS                      |                                      |                                                                                  |                                                          |
| <b>Nebulizer</b>                  | ESI 100 µL/min microFAST MC syringe injection autosampler  |                                      |                                                                                  |                                                          |
| <b>Cones</b>                      | X skimmer Ni cone, Jet sampler Ni cone                     |                                      |                                                                                  |                                                          |
| <b>Resolution</b>                 | Low                                                        |                                      |                                                                                  |                                                          |
| <b>Method</b>                     | 75 × 8s × 10 samples                                       |                                      |                                                                                  |                                                          |
| <b>Interference corrections</b>   | <sup>174</sup> Yb<br><sup>176</sup> Yb<br><sup>182</sup> W | <sup>204</sup> Hg                    | <sup>142</sup> Ce<br><sup>144</sup> Sm<br><sup>148</sup> Sm<br><sup>150</sup> Sm | <sup>84</sup> Kr<br><sup>86</sup> Kr<br><sup>87</sup> Rb |
| <b>Mass bias correction</b>       | <sup>179</sup> Hf/ <sup>177</sup> Hf                       | <sup>203</sup> Tl/ <sup>205</sup> Tl | <sup>146</sup> Nd/ <sup>144</sup> Nd                                             | <sup>88</sup> Sr/ <sup>86</sup> Sr                       |

Table 2. Cup configurations used for analysis of hafnium, lead, neodymium and strontium

|                  | L5                | L4                | L3                | L2                | L1                | C                 | H1                | H2                | H3                | H4                | H5                  |
|------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|---------------------|
| <b>Hafnium</b>   | <sup>172</sup> Yb | <sup>173</sup> Yb | <sup>174</sup> Hf | <sup>175</sup> Lu | <sup>176</sup> Hf | <sup>177</sup> Hf | <sup>178</sup> Hf | <sup>179</sup> Hf | <sup>180</sup> Hf | <sup>182</sup> W  | <sup>176</sup> Hf.O |
| <b>Lead</b>      | –                 | –                 | <sup>202</sup> Hg | <sup>203</sup> Tl | <sup>204</sup> Pb | <sup>205</sup> Tl | <sup>206</sup> Pb | <sup>207</sup> Pb | <sup>208</sup> Pb | –                 | –                   |
| <b>Neodymium</b> | <sup>140</sup> Ce | <sup>142</sup> Nd | <sup>143</sup> Nd | <sup>144</sup> Nd | <sup>145</sup> Nd | <sup>146</sup> Nd | <sup>147</sup> Sm | <sup>148</sup> Nd | <sup>149</sup> Sm | <sup>150</sup> Nd | <sup>142</sup> Nd.O |
| <b>Strontium</b> |                   | <sup>82</sup> Kr  | <sup>83</sup> Kr  | <sup>84</sup> Sr  | <sup>85</sup> Rb  | <sup>86</sup> Sr  | <sup>87</sup> Sr  | <sup>88</sup> Sr  | –                 | –                 | –                   |



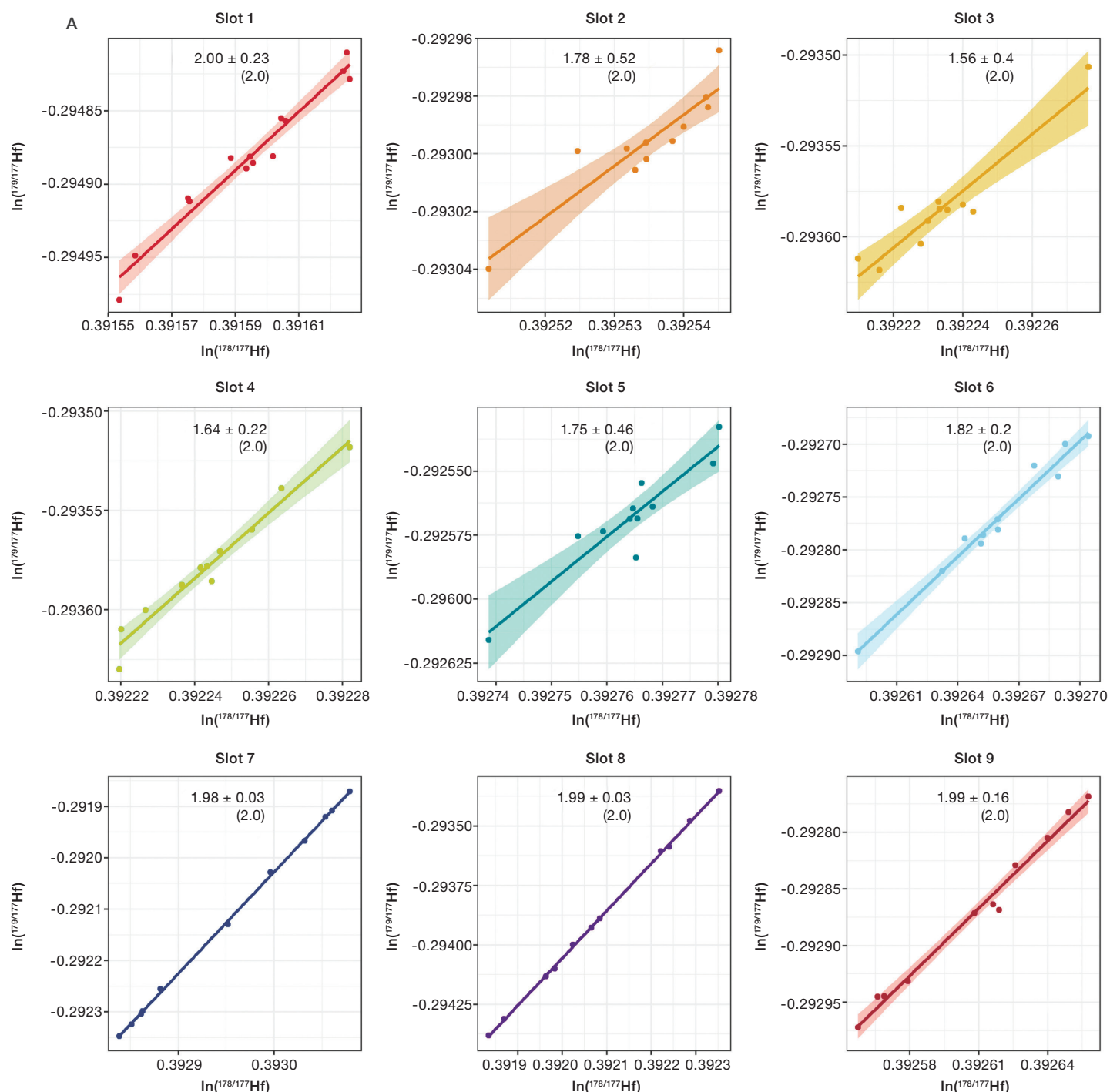
● Slot 1    ● Slot 2    ● Slot 3    ● Slot 4    ● Slot 5    ● Slot 6    ● Slot 7    ● Slot 8    ● Slot 9

**Figure 1. Sensitivities of 9 instruments tested within the factory.** Note that the instruments have only been crudely tuned to hit the sensitivity specification.

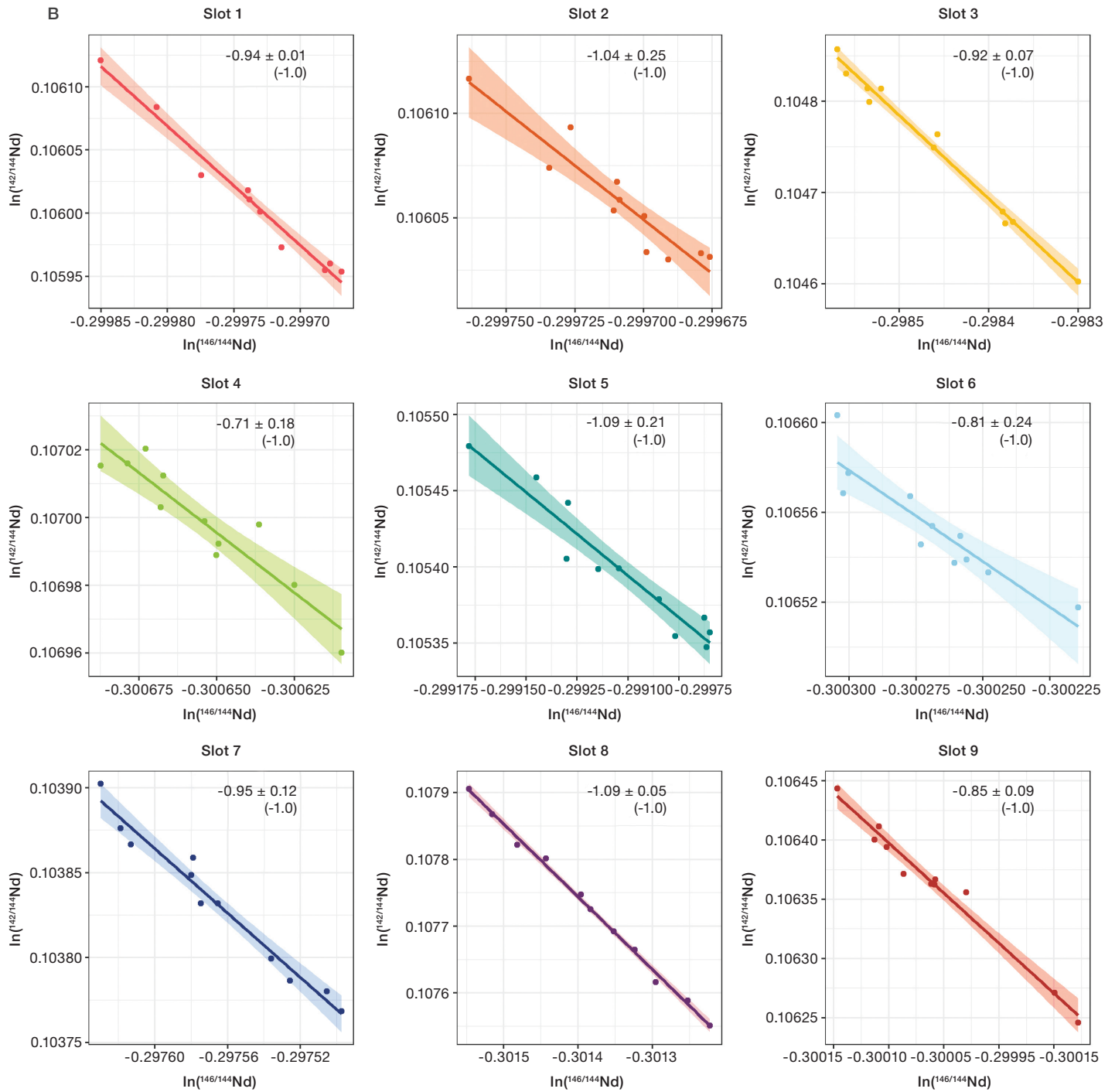
## Mass bias

Log-log plots were constructed to examine the mass bias behavior of the different isotope systems (Figure 2). All data plotted has been interference, but not mass bias corrected. All instruments display predictable exponential mass bias behavior in which the slope of the lines agrees with the predicted value (shown in brackets). The only cases where a slight deviation from the predicted value is observed are those instruments/analyses in which the range

of isotope ratios (on the x-axis) was relatively small. These cases can be identified as having a larger error envelope on the slope. However, where there is a reasonable range of isotope ratios, the slope follows exponential mass bias, demonstrating that it is appropriate to apply exponential mass bias corrections to data analyzed on Neoma MS/MS MC-ICP-MS.



**Figure 2. Log-log plots showing mass bias behavior of the 9 different instruments tested.** The slope and 2 sigma uncertainty are shown on each plot. The predicted value based on exponential law is shown in brackets below. (A) Hafnium, (B) Neodymium, (C) Lead, and (D) Strontium.



**Figure 2 continued. Log-log plots showing mass bias behavior of the 9 different instruments tested.** The slope and 2 sigma uncertainty are shown on each plot. The predicted value based on exponential law is shown in brackets below. (A) Hafnium, (B) Neodymium, (C) Lead, and (D) Strontium.

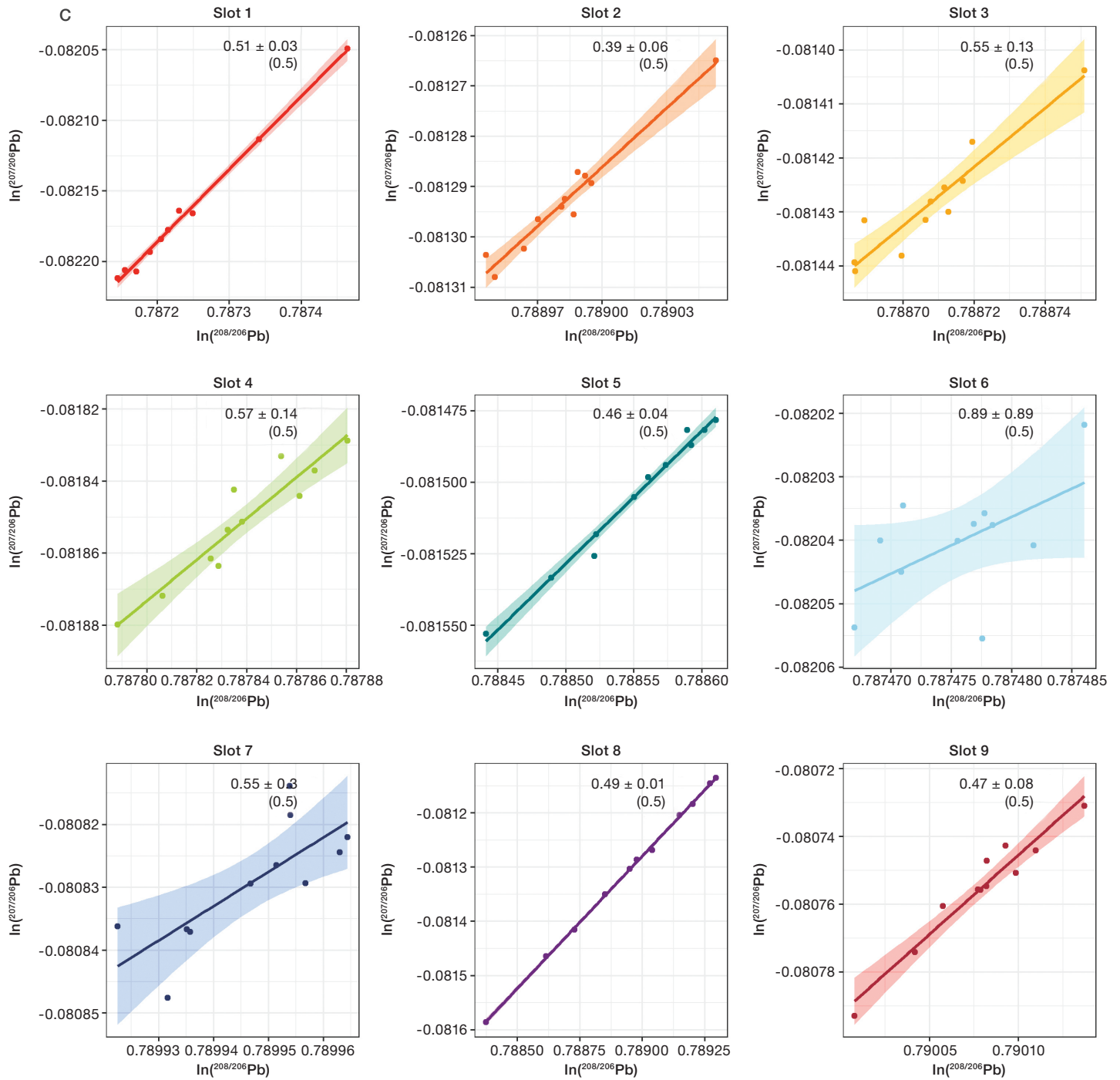
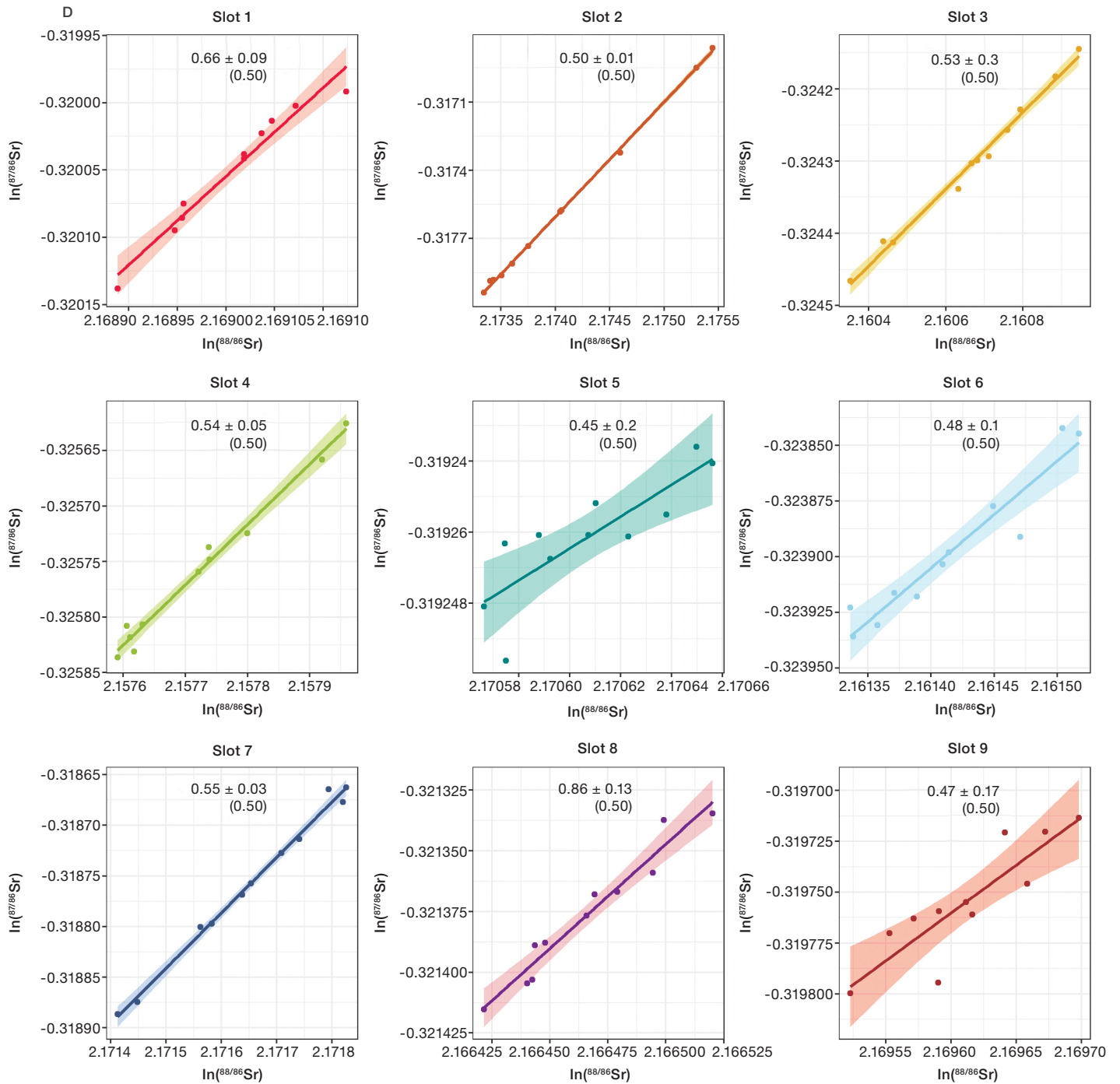


Figure 2 continued. Log-log plots showing mass bias behavior of the 9 different instruments tested. The slope and 2 sigma uncertainty are shown on each plot. The predicted value based on exponential law is shown in brackets below. (A) Hafnium, (B) Neodymium, (C) Lead, and (D) Strontium.

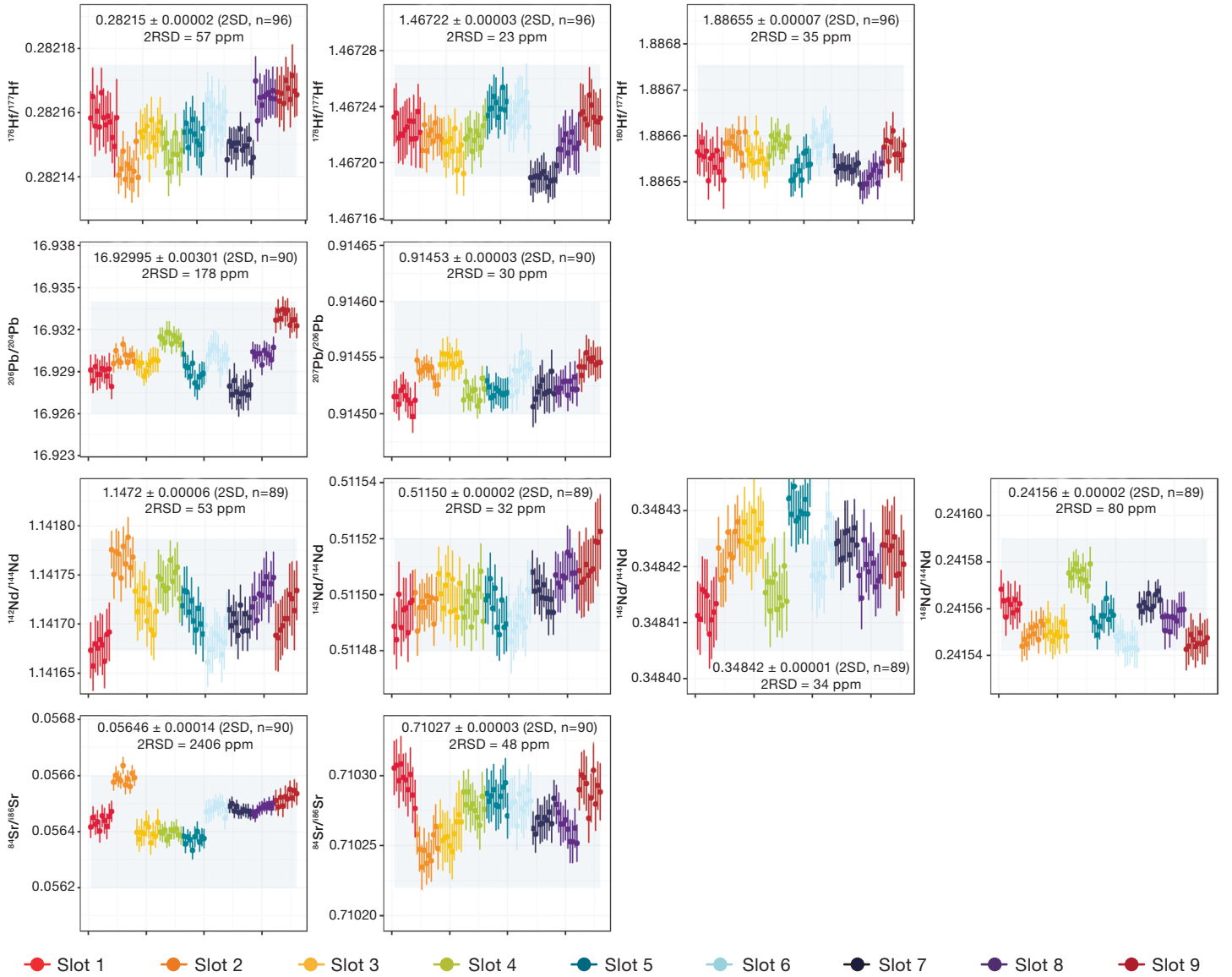


**Figure 2 continued. Log-log plots showing mass bias behavior of the 9 different instruments tested.** The slope and 2 sigma uncertainty are shown on each plot. The predicted value based on exponential law is shown in brackets below. (A) Hafnium, (B) Neodymium, (C) Lead, and (D) Strontium.

### Cross-instrument reproducibility

The accuracy and precision of the isotope ratios of the 4 known solutions was determined on each instrument (Figure 3). Internal and external precision on all determined isotope ratios is the same, and all isotope ratios fall within the expected value (gray box). The relative standard deviation of all ca. 100 analyses is relatively small (20-60 ppm) for all isotope ratios showing the good reproducibility of each individual Neoma MS/MS MC-ICP-MS<sup>1</sup>.

<sup>1</sup> Exceptions being  $^{204}\text{Pb}$  and  $^{84}\text{Sr}$  which are very low abundance, 1.4% and 0.56% respectively.



**Figure 3. Reproducibility of isotope ratios for each of the different isotopic systems (hafnium, lead, neodymium and strontium).** The data from each slot is shown in color. The expected value for the solution is shown as the grey rectangle. Note that samples are not standard-sample bracketed.

The internal and external precision of each set of analyses ( $n=10$ ) can be compared to the predicted precision based on counting statistics and Johnson-Niquist noise (Figure 4). The data fall close to the 1:1 line showing that we captured the two main sources of uncertainty.

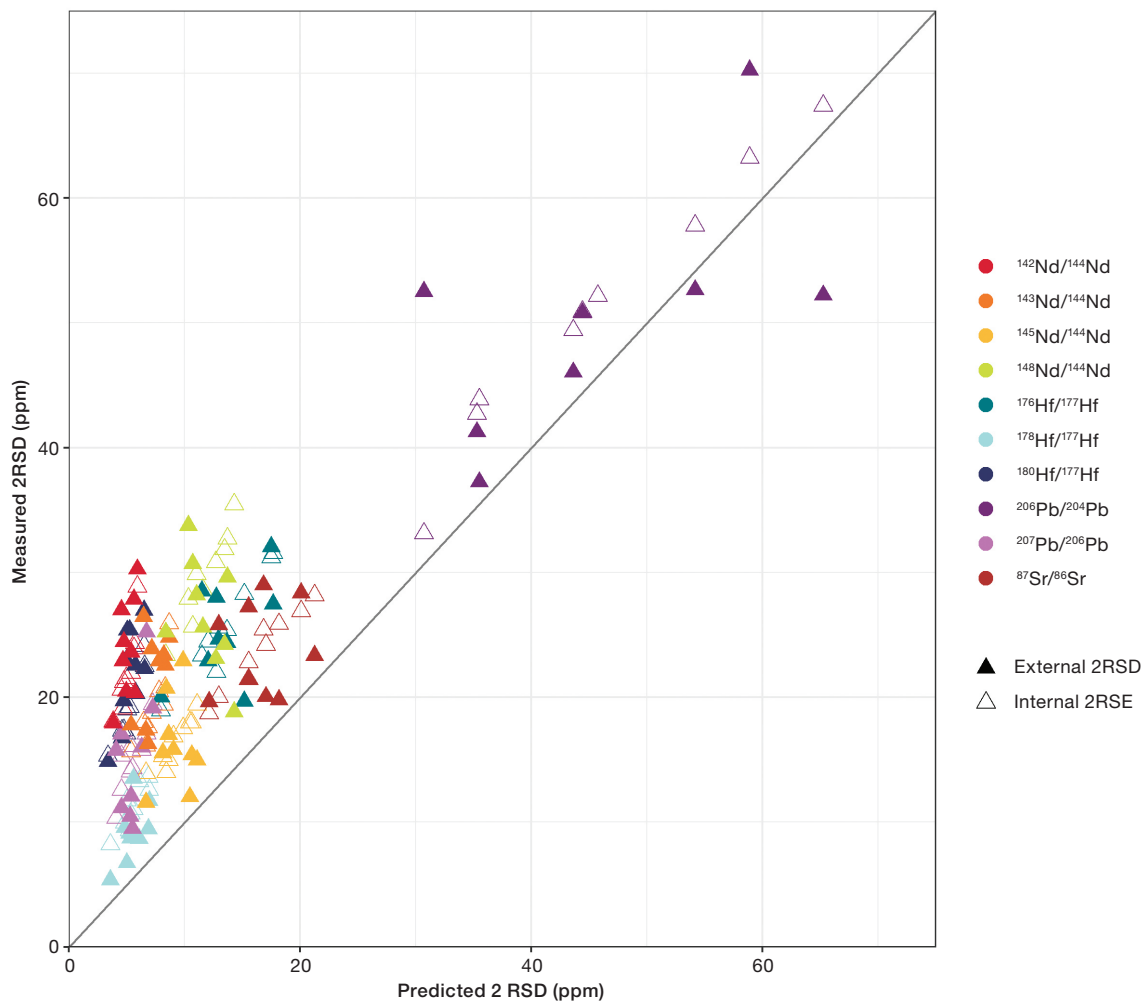


Figure 4. Comparison of the internal 2RSE (open symbols) and external 2RSD (closed symbol) for different isotope ratios against the predicted 2RSD based on counting statistics and Johnson-Niquist noise

## Conclusions

Isotopic data on hafnium, lead, neodymium and strontium was gathered from the Bremen factory on 9 different Neoma MS/MS MC-ICP-MS systems in full ion transmission mode with no collision/reaction cell gases. The key conclusions are:

- Mass bias on all isotope systems is exponential
- Unbracketed isotope ratios are accurate and precise with external precision mirroring internal precision
- Precision across different instruments is similar demonstrating the robustness of the system
- The main sources of analytical uncertainty are related to counting statistics and Johnson-Niquist noise

## Appendix

A1. Reproducibility of isotope ratios

| Slot | Ratio                             | Mean     | 2SD      | 2RSD (ppm) |
|------|-----------------------------------|----------|----------|------------|
| 1    | $^{176}\text{Hf}/^{177}\text{Hf}$ | 0.282158 | 9.00E-06 | 32.1       |
| 2    |                                   | 0.282143 | 8.00E-06 | 28.0       |
| 3    |                                   | 0.282153 | 7.00E-06 | 24.4       |
| 4    |                                   | 0.282148 | 8.00E-06 | 28.5       |
| 5    |                                   | 0.282153 | 7.00E-06 | 24.7       |
| 6    |                                   | 0.282158 | 8.00E-06 | 27.5       |
| 7    |                                   | 0.282149 | 6.00E-06 | 20.0       |
| 8    |                                   | 0.282165 | 6.00E-06 | 22.9       |
| 9    |                                   | 0.282166 | 6.00E-06 | 19.7       |
| 1    | $^{178}\text{Hf}/^{177}\text{Hf}$ | 1.467225 | 1.40E-05 | 9.5        |
| 2    |                                   | 1.467219 | 1.30E-05 | 9.1        |
| 3    |                                   | 1.467209 | 2.00E-05 | 13.5       |
| 4    |                                   | 1.467219 | 1.40E-05 | 9.6        |
| 5    |                                   | 1.467241 | 1.30E-05 | 8.7        |
| 6    |                                   | 1.467236 | 1.70E-05 | 11.7       |
| 7    |                                   | 1.467189 | 8.00E-06 | 5.4        |
| 8    |                                   | 1.467213 | 1.00E-05 | 6.7        |
| 9    |                                   | 1.467234 | 1.30E-05 | 8.7        |
| 1    | $^{180}\text{Hf}/^{177}\text{Hf}$ | 1.886547 | 5.10E-05 | 27.0       |
| 2    |                                   | 1.886581 | 4.30E-05 | 23.0       |
| 3    |                                   | 1.886554 | 4.80E-05 | 25.4       |
| 4    |                                   | 1.886584 | 3.20E-05 | 16.8       |
| 5    |                                   | 1.88653  | 4.80E-05 | 25.4       |
| 6    |                                   | 1.886593 | 4.20E-05 | 22.3       |
| 7    |                                   | 1.88653  | 2.80E-05 | 14.9       |
| 8    |                                   | 1.886512 | 3.70E-05 | 19.7       |
| 9    |                                   | 1.886571 | 4.30E-05 | 22.6       |
| 1    | $^{206}\text{Pb}/^{204}\text{Pb}$ | 16.92886 | 0.000891 | 52.7       |
| 2    |                                   | 16.93004 | 0.000889 | 52.5       |
| 3    |                                   | 16.92951 | 0.00078  | 46.1       |
| 4    |                                   | 16.93135 | 0.000631 | 37.3       |
| 5    |                                   | 16.92896 | 0.001391 | 82.2       |
| 6    |                                   | 16.93012 | 0.001189 | 70.3       |
| 7    |                                   | 16.92763 | 0.000884 | 52.2       |
| 8    |                                   | 16.93021 | 0.000699 | 41.3       |
| 9    |                                   | 16.93288 | 0.00086  | 50.8       |

A1 continued. Reproducibility of isotope ratios

| Slot | Ratio                             | Mean     | 2SD      | 2RSD (ppm) |
|------|-----------------------------------|----------|----------|------------|
| 1    | $^{207}\text{Pb}/^{206}\text{Pb}$ | 0.914513 | 1.50E-05 | 16.0       |
| 2    |                                   | 0.914537 | 1.40E-05 | 15.7       |
| 3    |                                   | 0.914548 | 1.00E-05 | 10.5       |
| 4    |                                   | 0.914518 | 1.60E-05 | 17.0       |
| 5    |                                   | 0.91452  | 9.00E-06 | 9.5        |
| 6    |                                   | 0.914535 | 2.30E-05 | 25.2       |
| 7    |                                   | 0.91452  | 1.80E-05 | 19.2       |
| 8    |                                   | 0.914524 | 1.00E-05 | 11.2       |
| 9    |                                   | 0.914545 | 1.10E-05 | 12.1       |
| 1    | $^{142}\text{Nd}/^{144}\text{Nd}$ | 1.141677 | 2.30E-05 | 20.4       |
| 2    |                                   | 1.141767 | 2.60E-05 | 22.9       |
| 3    |                                   | 1.141715 | 3.20E-05 | 27.9       |
| 4    |                                   | 1.141745 | 2.30E-05 | 20.5       |
| 5    |                                   | 1.141712 | 3.10E-05 | 27.0       |
| 6    |                                   | 1.141683 | 2.70E-05 | 23.6       |
| 7    |                                   | 1.141704 | 2.00E-05 | 17.9       |
| 8    |                                   | 1.141731 | 2.80E-05 | 24.5       |
| 9    |                                   | 1.141708 | 3.50E-05 | 30.3       |
| 1    | $^{143}\text{Nd}/^{144}\text{Nd}$ | 0.511492 | 1.20E-05 | 22.6       |
| 2    |                                   | 0.511496 | 9.00E-06 | 17.4       |
| 3    |                                   | 0.5115   | 1.20E-05 | 23.4       |
| 4    |                                   | 0.511497 | 1.20E-05 | 23.9       |
| 5    |                                   | 0.511495 | 1.40E-05 | 26.5       |
| 6    |                                   | 0.511492 | 1.20E-05 | 22.9       |
| 7    |                                   | 0.5115   | 9.00E-06 | 17.8       |
| 8    |                                   | 0.511507 | 8.00E-06 | 16.3       |
| 9    |                                   | 0.511511 | 1.30E-05 | 24.8       |
| 1    | $^{145}\text{Nd}/^{144}\text{Nd}$ | 0.348412 | 5.00E-06 | 15.4       |
| 2    |                                   | 0.348423 | 7.00E-06 | 20.7       |
| 3    |                                   | 0.348426 | 4.00E-06 | 12.0       |
| 4    |                                   | 0.348415 | 6.00E-06 | 15.8       |
| 5    |                                   | 0.348431 | 5.00E-06 | 15.6       |
| 6    |                                   | 0.348422 | 8.00E-06 | 22.9       |
| 7    |                                   | 0.348424 | 4.00E-06 | 11.6       |
| 8    |                                   | 0.348419 | 6.00E-06 | 17.0       |
| 9    |                                   | 0.348423 | 5.00E-06 | 15.0       |

**A1 continued. Reproducibility of isotope ratios**

| Slot | Ratio                           | Mean     | 2SD      | 2RSD (ppm) |
|------|---------------------------------|----------|----------|------------|
| 1    | $^{84}\text{Sr}/^{86}\text{Sr}$ | 0.056437 | 4.30E-05 | 766.6      |
| 2    |                                 | 0.05659  | 4.30E-05 | 758.1      |
| 3    |                                 | 0.056397 | 4.70E-05 | 828.6      |
| 4    |                                 | 0.056394 | 2.50E-05 | 449.8      |
| 5    |                                 | 0.056372 | 3.70E-05 | 652.1      |
| 6    |                                 | 0.056481 | 3.20E-05 | 559.5      |
| 7    |                                 | 0.056478 | 2.40E-05 | 423.5      |
| 8    |                                 | 0.056483 | 2.80E-05 | 496.9      |
| 9    |                                 | 0.056521 | 4.20E-05 | 743        |
| 1    | $^{87}\text{Sr}/^{86}\text{Sr}$ | 0.710297 | 2.00E-05 | 28.4       |
| 2    |                                 | 0.710248 | 1.90E-05 | 27.2       |
| 3    |                                 | 0.710259 | 1.70E-05 | 23.4       |
| 4    |                                 | 0.710278 | 1.50E-05 | 21.5       |
| 5    |                                 | 0.710284 | 1.40E-05 | 20.1       |
| 6    |                                 | 0.710279 | 1.40E-05 | 19.8       |
| 7    |                                 | 0.710268 | 1.40E-05 | 19.6       |
| 8    |                                 | 0.710263 | 1.80E-05 | 25.8       |
| 9    |                                 | 0.71029  | 2.10E-05 | 29.0       |

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