High-Throughput Method for Strontium Isotope Analysis by Multi-Collector-Inductively Coupled Plasma-Mass Spectrometer

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Cover Illustration: Multi-collector inductively-coupled plasma-mass spectrometer.


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https://edx.netl.doe.gov/ucr
High-Throughput Method for Strontium Isotope Analysis by Multi-Collector-Inductively Coupled Plasma-Mass Spectrometer

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# Table of Contents

**EXECUTIVE SUMMARY** ...........................................................................................................1

1. **INTRODUCTION** ................................................................................................................2

2. **HIGH-THROUGHPUT STRONTIUM SEPARATION PROCEDURE** ..................................4
   2.1 MATERIALS AND SAMPLE PREPARATION ............................................................4
   2.2 COLUMN CONFIGURATION ......................................................................................4
   2.3 MATERIALS PREP ........................................................................................................6
   2.4 COLUMN CLEANING ...................................................................................................6
   2.5 RESIN ADDITION AND CLEANING ..........................................................................6
   2.6 RESIN CONDITIONING ..............................................................................................6
   2.7 SAMPLE LOADING .....................................................................................................7
   2.8 RINSING MATRIX ......................................................................................................7
   2.9 STRONTIUM ELUTIONS ..............................................................................................7
   2.10 PREPARATION FOR STRONTIUM ANALYSIS ........................................................7

3. **STRONTIUM SEPARATION PERFORMANCE** ..................................................................8
   3.1 STRONTIUM SEPARATION FROM RUBIDIUM .......................................................8
   3.2 STRONTIUM SEPARATION FROM MATRIX ELEMENTS .........................................8
   3.3 MATRIX EFFECTS ON STRONTIUM YIELDS .............................................................10

4. **MC-ICP-MS OPTIMIZATION FOR STRONTIUM ISOTOPE MEASUREMENTS** ..........12

5. **COMPARISON OF MC-ICP-MS AND THERMAL IONIZATION MASS SPECTROMETRY** .................................................................................................................16

6. **DATA HANDLING AND REDUCTION** ............................................................................18
   6.1 INSTRUMENTAL MASS BIAS CORRECTIONS ..........................................................18
   6.2 DATA REDUCTION AND QUALITY ASSURANCE .....................................................18

7. **CONCLUSIONS** ...............................................................................................................19

8. **REFERENCES** ..................................................................................................................21

**APPENDIX A: DATA MANAGEMENT EXAMPLE OUTPUT** ............................................... A-1

**APPENDIX B: STRONTIUM ISOTOPE DATA REDUCTION FOR THERMO NEPTUNE** ........ B-1

**APPENDIX C: EXCEL MACRO** .......................................................................................... C-1
List of Figures

Figure 1: NETL’s Thermo Scientific NEPTUNE PLUS MC-ICP-MS at the University of Pittsburgh, Department of Geology and Planetary Science ................................................................. 2
Figure 2: Sr separation column assembly for vacuum extraction .......................................................................................................................... 5
Figure 3: Vacuum box for Sr separation chemistry. The box can accommodate up to 24 samples per batch. ......................................................................................................................... 5
Figure 4: Elution curves showing the typical separation of Rb from Sr in a clean matrix .......... 8
Figure 5: Elution curves showing the separation of Sr (2 µg) from Rb (1 µg) with a complex matrix of Ca, K, Ba, and Fe (at 871, 47, 4.7 and 1,147 µg, respectively) ..................................................... 10
Figure 6: Sr recoveries from columns loaded with Ca, K, Ba, and Fe. 2 µg Sr, 1 µg Rb, and the matrix element were added to the column and Sr yields were measured in the water elution step. ............................................................................................................. 11
Figure 7: Measured value of NIST SRM 987 plotted against the voltage of $^{88}$Sr. Error bars indicate the in-run standard error of NIST 987 $^{87}$Sr/$^{86}$Sr at various solution concentrations and instrument settings. Solution of NIST 987 with [Sr] of 100 ppb, 200 ppb, 300 ppb, 400 ppb, and 500 ppb were run using the same instrument settings. NIST 987 solutions of 400 and 500 ppb were run while detuning the instrument (lowered sample gas). ............................. 14
Figure 8: $^{87}$Sr/$^{86}$Sr values of repeat measurement of NIST 987 over 2 weeks. The average value is 0.710265 ± 14 (2σ) ............................................................................................................. 15
Figure 9: Differences in $^{87}$Sr/$^{86}$Sr values measured by the University of Pittsburgh TIMS and MC-ICP-MS vs. the average $^{87}$Sr/$^{86}$Sr values normalized to a common value for SRM 987 of 0.710240. The error bars represent the propagated error of both measurements. The bold dashed line represents the 2σ error (±0.000018, n = 10) and the light dashed line is the average difference of the $^{87}$Sr/$^{86}$Sr values (1.7x10^-6). ......................................................................................... 17

List of Tables

Table 1: Geochemistry and Sr isotope ratios of energy related fluids .................................................. 9
Table 2: MC-ICP-MS running parameters ............................................................................................ 13
# Acronyms, Abbreviations, and Symbols

<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
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</thead>
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<tr>
<td>DOE</td>
<td>U.S. Department of Energy</td>
</tr>
<tr>
<td>MC-ICP-MS</td>
<td>Multi-collector-inductively coupled plasma-mass spectrometer</td>
</tr>
<tr>
<td>MVA</td>
<td>Monitoring, verification, and accounting</td>
</tr>
<tr>
<td>NETL</td>
<td>National Energy Technology Laboratory</td>
</tr>
<tr>
<td>SIS</td>
<td>Stable introduction system</td>
</tr>
<tr>
<td>Sr</td>
<td>Strontium</td>
</tr>
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<td>TIMS</td>
<td>Thermal ionization mass spectrometry</td>
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<td>Rb</td>
<td>Rubidium</td>
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Acknowledgments

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EXECUTIVE SUMMARY

This technical report highlights a new method for high-throughput strontium (Sr) separation chemistry and isotopic analysis by multi-collector-inductively coupled plasma-mass spectrometer (MC-ICP-MS). This method was developed for the specific task of separating Sr from water with complex matrices from geologic settings, while taking advantage of the increased throughput of vacuum methods. This method is optimized for purposes of using Sr isotopes for monitoring, verification, and accounting (MVA) related to geologic CO$_2$ storage and for the long-term monitoring of brine migration and fluid/rock reactions related to oil/natural gas production. This technique potentially offers an order of magnitude improvement in speed compared to traditional methods. The benefits of this method over other separation protocols include:

1) Cost savings – the modifications of this method to current vacuum assisted Sr extraction techniques reduces the resin reservoir and reagents used for cost savings

2) Disposability – this design eliminates the concern for residual contaminants

3) Ease of use – column components consist of off-the-shelf, easy to obtain, parts

4) Optimization for specific matrix effects – specific interference elements have been accounted for that are common in formation waters and related fluids that could influence Sr yields (e.g. Ba, Ca, K, Fe)

5) Optimization for MC-ICP-MS – this method is designed for immediate isotopic analysis of Sr separated by MC-ICP-MS with no additional evaporation step

This technical report presents the details of the Sr column configuration and the high-throughput Sr separation protocol. Data showing the performance of the method as well as the best practices for optimizing Sr isotope analysis by MC-ICP-MS is presented. Lastly, this report offers tools for data handling and data reduction of Sr isotope results from the Thermo Scientific Neptune software to assist in data quality assurance, which help avoid issues of data glut associated with high sample throughput rapid analysis.

A concise version of this report has been published in a peer reviewed journal, Journal of Analytical Atomic Spectrometry (Wall et al., 2013).
1. **INTRODUCTION**

Strontium (Sr) isotopes have been proven to be a sensitive natural tracer useful for monitoring fluid-rock interactions and for tracking the origin of dissolved solids in surface and ground water systems (Banner, 2004). Because $^{87}\text{Sr}$ is a radiogenic, i.e. a relatively high-mass isotope produced by the decay of $^{87}\text{Rb}$, variation in the isotopic ratio of $^{87}\text{Sr}/^{86}\text{Sr}$ due to natural fractionation processes (e.g., temperature, biological activity, and evaporation) can be neglected, in contrast to lower mass systems such as C, O, and H (Capo et al., 1998). The $^{87}\text{Sr}/^{86}\text{Sr}$ isotope ratio is useful for studying the migration of formation brines into surface and groundwater (Barnaby et al., 2004; Campbell et al., 2008; Chapman et al., 2012; Osborn et al., 2012), the interaction of coal fly ash with acid mine drainage (Hamel et al., 2010; Spivak-Birndorf et al., 2012), subsurface fluid flow in oil/natural gas reservoirs (Barnaby et al., 2004; Osborn et al., 2012), and fluid/rock reactions related to geologic storage of carbon dioxide (CO$_2$) (Quattrocchi et al., 2006).

Sr isotope analysis can be achieved by either using thermal ionization mass spectrometry (TIMS) or multi-collector-inductively coupled plasma-mass spectrometer (MC-ICP-MS) (Figure 1), which is a newly established method that allows for higher sample throughput (Fortunato et al., 2004; Vanhaecke et al., 2009). However, accurate and precise Sr isotope measurements by either technique require the separation of isoobaric interferences (mainly Rb) and the removal of matrix elements (Balcaen et al., 2005; Becker, 2005; Pin et al., 2003). Strontium is routinely separated from sample matrices using Sr specific extraction resins loaded onto chromatographic columns (Horwitz et al., 1992; Horwitz et al., 1991). While these gravity flow methods are extremely effective at purifying aqueous samples for Sr, they can be time consuming.

![Figure 1: NETL’s Thermo Scientific NEPTUNE PLUS MC-ICP-MS at the University of Pittsburgh, Department of Geology and Planetary Science.](image)

In order for Sr isotopes to serve as a useful tool for long-term monitoring of fluid migration related to oil and natural gas production or for monitoring, verification, and accounting (MVA) of CO$_2$ storage, rapid Sr separations methods are required. Improvements to gravity flow separation methods have come with the development of coupled chromatographic/MC-ICP-MS
techniques and vacuum assisted methods (EPA, 2010; Galler et al., 2008; Garcia-Ruiz et al., 2008; Maxwell, 2006; Maxwell et al., 2010). Coupled methods use ion chromatographs attached directly to mass spectrometers (Galler et al., 2008; Garcia-Ruiz et al., 2008). These methods result in high sample throughput, but their benefit can only be realized in the presence of a MC-ICP-MS, eliminating the option for TIMS analysis or offsite sample processing. Alternatively, vacuum assisted Sr separation can be carried out anywhere there is a clean laminar flow hood. However, these vacuum extraction techniques require large, expensive resin cartridges, and current vacuum-based techniques are designed specifically for evaluation of radioactive Sr in environmental samples and have not been optimized specifically for isotope ratio measurement of the eluted Sr in terms of procedural blanks and proper concentrations for analysis by MC-ICP-MS (Maxwell, 2006; Maxwell et al., 2010).

This technical report highlights a new method for high-throughput Sr separation chemistry and isotopic analysis by MC-ICP-MS. The method was developed for the specific task of separating Sr from water with complex matrices from geologic settings while taking advantage of the increased throughput of vacuum methods. This method is optimized for purposes of using Sr isotopes for MVA related to geologic CO$_2$ storage and for the long-term monitoring of brine migration and fluid/rock reactions related to oil/natural gas production. The benefits of this method over other separation protocols include:

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2) *Disposability* – this design eliminates the concern for residual contaminants

3) *Ease of use* – column components consist of off-the-shelf, easy to obtain, parts

4) *Optimization for specific matrix effects* – specific interference elements have been accounted for that are common in formation waters and related fluids that could influence Sr yields (e.g. Ba, Ca, K, Fe)

5) *Optimization for MC-ICP-MS* – this method is designed for immediate isotopic analysis of Sr separate by MC-ICP-MS with no additional evaporation step

This technical report presents the details of the Sr column configuration and the high-throughput Sr separation protocol. Data showing the performance of the method as well as the best practices for optimizing Sr isotope analysis by MC-ICP-MS is presented. Lastly, this report offers tools for data handling and data reduction of Sr isotope results from the Thermo Scientific Neptune software to assist in data quality assurance help avoid issues of data glut associated with high sample throughput rapid analysis.

A concise version of this report has been published in a peer reviewed journal, *Journal of Analytical Atomic Spectrometry* (Wall et al., 2013).
2. HIGH-THROUGHPUT STRONTIUM SEPARATION PROCEDURE

2.1 MATERIALS AND SAMPLE PREPARATION

During the development of this method all sample handling was done in Class 100 vertical laminar flow hoods. Ultrapure nitric acid (HNO₃) (e.g. Optima, Fisher Chemical, USA) is required for sample acidification, resin/column cleaning, and elutions to prevent Sr contamination. Ultrapure 18.2 MΩ·cm water (MQW) (e.g. Milli-Q, Millipore, USA) is also necessary for acid dilution, resin cleaning, and Sr elution. The Sr specific resin (Horwitz et al., 1991) (50–100 μm particle size) (Sr-resin®, Eichrom Technologies, Inc., USA) must be pre-cleaned prior to use with 8N HNO₃ and Milli-Q water (Smet et al., 2010). Before undertaking separation procedures, samples are to be filtered to <0.45 μm and then acidified with concentrated nitric acid to produce at 2% (v/v) nitric acid solution. Strontium concentrations of each sample must be obtained before proceeding to the separation procedure in order to calculate the proper volume of sample to evaporate in order to obtain 2 μg Sr. Lastly, in order to prevent contamination, samples should be evaporated in acid washed Teflon in a clean hood.

2.2 COLUMN CONFIGURATION

The column assembly (Figure 2) consists of a 3 mL syringe reservoir (National Scientific Co., part # S7515-3) attached via Luer Lock fitting to a 700 μL microcolumn (MoBiTec GmbH, part # M105010S). Sr-resin® is loaded into the microcolumn and fitted into the inner and outer tips (Eichrom Technologies, LLC, part #AC-1000-IT, OT) that are inserted into the vacuum box. All parts of the column assembly are acid cleaned before use. The polycarbonate vacuum box (Figure 3) (Eichrom Technologies, LLC) can accommodate 24 samples and is described in more detail (Maxwell, 2006). A vacuum pump that is capable of achieving a pressure of ~15 in. Hg is required for this protocol (e.g. Gast 1/6 hp Reciprocating Pump, #1HAB25M100X).
Figure 2: Sr separation column assembly for vacuum extraction (Wall et al., 2013).

Figure 3: Vacuum box for Sr separation chemistry. The box can accommodate up to 24 samples per batch.
2.3 MATERIALS PREP

2.3.1 Prior to using the vacuum box, rinse it with MQW and allow it to dry thoroughly.

2.3.2 Add 300 µL of MQW water to 700 µL microcolumn using a pipette; mark columns with a dot at the top of the 300 µL level. Discard the water.

2.3.3 Add 0.25 mL 8 N HNO₃ to the Teflon vials containing the evaporated samples (containing 2 µg Sr). Add additional 0.25 mL if necessary to dissolve dried residue. Another 0.25 mL can be added, but the total volume of 8N HNO₃ should NOT exceed 0.75 mL of 8 N HNO₃. If the sample cannot be taken up in 8 N HNO₃, exclude that sample from the procedure. Note the volume added to each sample in lab notes.

2.4 COLUMN CLEANING

2.4.1 Place waste container in vacuum box.

2.4.2 Attach microcolumn to the white and yellow vacuum box tips. Do not attach luer lock cap or reservoir at this time. Label samples on top of vacuum box and insert column assembly into the holes.

2.4.3 Add small amount of water to the microcolumn to wet frit and ensure that the column will flow. Turn on pump and keep at maximum pressure (~10–15 in. Hg).

2.4.4 Fill to the top of the microcolumn with MQW and pump through.

2.4.5 Turn off the pump. Fill to the top of the microcolumn with 8 N HNO₃ and let it sit for 60 s. Turn on pump and pump the acid through the microcolumn.

2.4.6 Fill column to the top of the microcolumn with MQW and pump through.

2.5 RESIN ADDITION AND CLEANING

2.5.1 Shake the resin bottle to make sure the resin is well mixed. WITH PUMP RUNNING AT MAXIMUM PRESSURE (~ 10–15 in. Hg), use a pipettor to load resin. Load the resin a few drops at a time until the resin bed reaches the 300 µL mark. The goal is to make a resin bed that is as compact as possible to prevent channeling.

2.5.2 With the pump running, connect the luer lock fitting and reservoir to each microcolumn.

2.5.3 With the pump running, add 3 mL of 8N HNO₃ to the reservoir and pump liquid through columns.

2.5.4 Add 3 mL of MQW in the same manner as in Step 2.5.3.

2.5.5 Repeat Step 2.5.3 once.

2.5.6 Repeat Step 2.5.4 once.

2.6 RESIN CONDITIONING

2.6.1 Add 3 mL of 8 N HNO₃ to the reservoir. Reduce pressure using the vacuum box valve and calibrate flow rate to ≤ 1 mL/min, typically between 4 and 5 in Hg. Add
an additional 2 mL of 8 N HNO₃ before the resin dries. Ensure that the flow rate is ≤ 1 mL/min. Note the pressure for this flow rate in lab notes.

2.6.2 Let the pump run until all of HNO₃ is out of the resin.

2.7 SAMPLE LOADING
2.7.1 Turn off the pump.
2.7.2 Inspect each sample to make sure it is fully dissolved in 8 N HNO₃.
2.7.3 Using a new, clean pipette tip for each sample, pipette the dissolved sample into the reservoir. DO THIS VERY SLOWLY, DOWN THE SIDE OF THE RESERVOIR AND AS CLOSE TO THE BOTTOM OF THE RESERVOIR AS POSSIBLE. Pipetting directly into the bottom will create channels.
2.7.4 Turn on pump and draw sample through the resin.

2.8 RINSING MATRIX
2.8.1 Use a squeeze bottle with 8 N HNO₃ for the following steps. To avoid sample contamination, make sure the tip of the bottle does not make contact with any of the reservoir sides. If the sample has low [Sr] or is a sensitive sample, collect these matrix rinses separately from the elutions.
2.8.2 Add 0.5 mL of 8 N HNO₃ to each reservoir and pump through at ≤ 1 mL/min.
2.8.3 Next add 1 mL of 8 N HNO₃.
2.8.4 Next add 2 ml of 8 N HNO₃.
2.8.5 Near end of the rinse, increase the pressure to around 10 in Hg to ensure that all of HNO₃ has passed through the columns.
2.8.6 Turn off the pump and remove the waste container.

2.9 STRONTIUM ELUTIONS
2.9.1 Label 15 mL centrifuge tubes with sample name and place each one in the corresponding spot in the centrifuge rack.
2.9.2 Install centrifuge rack for sample collection.
2.9.3 Using the MQW squeeze bottle, add 2 mL of MQW to each reservoir as precisely as possible. Turn on pump so flow through column is ≤ 1 mL/min.
2.9.4 Add an additional 2 mL of MQW as precisely as possible.
2.9.5 Once elution is complete, increase the pressure to ensure that all of MQW has passed through the columns and you have collected the totality of the sample.

2.10 PREPARATION FOR STRONTIUM ANALYSIS
2.10.1 Spike the eluted sample (4 mL MQW) with 80 μL of UP conc HNO₃ to make a 2% solution for analysis by MC-ICP-MS.
3. STRONTIUM SEPARATION PERFORMANCE

3.1 STRONTIUM SEPARATION FROM RUBIDIUM

To ensure that this method can adequately separate Rb from Sr, 2 μg Sr and 1μg Rb were loaded onto the column and the eluted fractions were collected and analyzed for Rb and Sr. Rubidium was ~100% eluted after 2 mL of 8 N HNO₃. An additional 2 mL of 8 N HNO₃ was added to ensure that the tail of the Rb elution curve returned to background. Maximum recovery of Sr was achieved with the addition of 4 mL of Milli-Q H₂O. Figure 4 shows the elution curves for one experiment with an 88% Sr yield. Less than 100% Sr yields are not atypical and recoveries as low as 70% have been reported (Charlier et al., 2006). Even if Sr isotopes are fractionated on the column, the exponential correction for mass bias that was employed when the data was reduced eliminates the influence of any variations in \(^{88}\)Sr/\(^{86}\)Sr. While it is important to have high Sr yields in order to maintain proper signal strength for MC-ICP-MS measurements, the exponential correction precludes the need for 100% recovery Sr to achieve accurate \(^{88}\)Sr/\(^{86}\)Sr ratios.

![Figure 4: Elution curves showing the typical separation of Rb from Sr in a clean matrix (Wall et al., 2013).](image)

3.2 STRONTIUM SEPARATION FROM MATRIX ELEMENTS

To demonstrate that the Sr separation procedure can effectively isolate Sr from matrix elements known to interfere with column yield (Horwitz et al., 1992; Horwitz et al., 1991) or MC-ICP-MS analysis (Rb), columns were loaded with 2 μg Sr, 1μg Rb, and a range of Ca, K, Ba, and Fe at molar ratios equivalent to what is observed for a variety of energy related geofluids (Table 1). These fluids include fly ash impoundment waters, acid mine drainage, formation brines, Marcellus shale produced waters, and fluids associated with geologic analogs for carbon storage.
For the elution experiment shown in Figure 5, the Sr and Rb mixture was spiked with 442 µg Ca, 4 µg K, 4 µg Ba, and 830 µg Fe which represent the highest element/Sr ratio in the samples from Table 1. Even with a complex matrix, Rb and Sr were separated effectively, with nearly all the Rb removed after addition of 2 mL of 8 N HNO₃. Ca, K, and Fe behaved similarly to Rb and were rinsed from the resin with 2 mL of 8 N HNO₃. Barium, on the other hand, is retained longer on the resin even when as much as 4 mL of 8 N HNO₃ is added. However, this behavior does not affect the elution of Rb or Sr. In fact, the Sr yield is similar (87% recovery) to the simple elution curve shown in Figure 4.

Table 1: Geochemistry and Sr isotope ratios of energy related fluids (Wall et al., 2013)

<table>
<thead>
<tr>
<th>Source</th>
<th>µS/cm</th>
<th>Ca/Sr</th>
<th>Ba/Sr</th>
<th>K/Sr</th>
<th>Fe/Sr</th>
<th>⁸⁷Sr/⁸⁶Sr ** ± 2(SE)</th>
<th>MC-ICP-MS</th>
<th>TIMS* - (MC-ICP-MS)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal ash storage impoundment</td>
<td>533</td>
<td>267</td>
<td>--</td>
<td>53.0</td>
<td>3.20</td>
<td>0.712927 12 ± 0.000015</td>
<td></td>
<td></td>
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<tr>
<td>Coal ash storage impoundment</td>
<td>561</td>
<td>301</td>
<td>--</td>
<td>45.0</td>
<td>--</td>
<td>0.712771 12 ± 0.000005</td>
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<tr>
<td>Abandoned natural gas well</td>
<td>1,275</td>
<td>633</td>
<td>0.08</td>
<td>38.0</td>
<td>913.0</td>
<td>0.715864 11 ± 0.000003</td>
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<td>Coal mine drainage (acidic)</td>
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<td>953</td>
<td>0.11</td>
<td>37.0</td>
<td>20.0</td>
<td>0.714503 11 ± 0.000013</td>
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<tr>
<td>Coal mine drainage (net alkaline)</td>
<td>--</td>
<td>136</td>
<td>0.04</td>
<td>3.6</td>
<td>31.18</td>
<td>0.712056 30 ± 0.000001</td>
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<tr>
<td>Formation brine</td>
<td>173,438</td>
<td>154</td>
<td>0.02</td>
<td>2.0</td>
<td>0.03</td>
<td>0.717022 11 ± 0.000005</td>
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<td></td>
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<tr>
<td>Hydraulic fracturing produced water</td>
<td>240,625</td>
<td>7</td>
<td>5.13</td>
<td>0.1</td>
<td>0.04</td>
<td>0.710742 5 ± 0.000009</td>
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</tr>
<tr>
<td>Hydraulic fracturing produced water</td>
<td>294,063</td>
<td>9</td>
<td>2.23</td>
<td>0.3</td>
<td>0.02</td>
<td>0.711173 5 ± 0.000008</td>
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<tr>
<td>High CO₂ natural analog</td>
<td>1,868</td>
<td>147</td>
<td>0.02</td>
<td>14.0</td>
<td>0.07</td>
<td>0.709566 10 ± 0.000009</td>
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<tr>
<td>High CO₂ natural analog</td>
<td>1,692</td>
<td>152</td>
<td>0.02</td>
<td>14.0</td>
<td>0.01</td>
<td>0.709544 7 ± 0.000008</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Source of TIMS data indicated by reference superscript
** TIMS and MC-ICP-MS values are normalized to SRM 987 = 0.71024
3.3 MATRIX EFFECTS ON STRONTIUM YIELDS

In order to better assess the influence of matrix elements on Sr recovery from the Sr-Resin®, columns were loaded with a solution containing 2 µg Sr, 1 µg Rb, and varying amounts of a single matrix element, including Ca (200–75,000 µg), K (10–4,000 µg), Ba (2–400 µg), and Fe (300–50,000 µg). The highest matrix element:Sr ratio of these solutions greatly exceed ratios measured in typical brine and produced water samples, in order to demonstrate the range of effectiveness of the column procedure to adequately separate Sr from a complex matrix, including brines.

Strontium yields using this method appear generally unaffected by increasing amounts of Fe and K (Figure 6). The result of the Fe experiment is not surprising as the binding efficiency of Fe on the resin is relatively low (Horwitz et al., 1992). However, high concentrations of K and Ca have been shown to reduce Sr retention (Horwitz et al., 1992). This study hypothesized that the higher nitric acid concentration, 8N compared to 3N used in Horwitz et al. (1992), in this method allows for better retention of Sr in the presence of these two elements. The Sr yield does begin to decrease with excessive amounts of Ca. However, this effect is observed when the Ca:Sr exceeds 20,000, roughly 20 times the ratio observed in these samples.
Figure 6: Sr recoveries from columns loaded with Ca, K, Ba, and Fe. 2 µg Sr, 1 µg Rb, and the matrix element were added to the column and Sr yields were measured in the water elution step. The vertical dashed line represents a typical ratio for produced water samples.

An increased amount of Ba in the matrix does apparently result in a reduction in Sr retention (Figure 6). The effect of Ba, however, occurs on these columns when the Ba:Sr is > 100:1. Even though produced waters from the Marcellus Shale have high Ba content (Table 1), the Ba:Sr ratio is < 6:1 indicating that this column method can effectively separate typical geological samples.
4. **MC-ICP-MS OPTIMIZATION FOR STRONTIUM ISOTOPE MEASUREMENTS**

Strontium isotope ratios were analyzed using a Thermo Scientific Neptune Plus double-focusing MC-ICP-MS (Thermo Scientific, Bremen, Germany) (Figure 1). Acidified solutions were introduced into a stable introduction system (SIS) spray chamber via a 100 μL/min PFA-nebulizer. Instrument parameters and cup configuration for Sr isotope ratio determination are summarized in Table 2. Operating conditions for Sr analysis by MC-ICP-MS were optimized to achieve a balance between precise and accurate isotope ratio measurements and high sample throughput. The goal in the column procedure was to obtain samples that were preserved and ready for immediate isotopic analysis, without an evaporation step. With that this study set out to determine the lowest Sr concentration necessary to achieve accurate and precise Sr isotope measurements using standard instrument settings.
Table 2: MC-ICP-MS running parameters

<table>
<thead>
<tr>
<th>Thermo Scientific Neptune Plus MC-ICP-MS</th>
<th>Typical Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>Running Parameter</td>
<td>Typical Setting</td>
</tr>
<tr>
<td>RF power</td>
<td>1,200 W</td>
</tr>
<tr>
<td>Cooling gas flow rate</td>
<td>15 L/min</td>
</tr>
<tr>
<td>Auxiliary gas flow rate</td>
<td>0.7 L/min</td>
</tr>
<tr>
<td>Sample gas flow rate</td>
<td>1.0 to 1.1 L/min</td>
</tr>
<tr>
<td>Extraction voltage</td>
<td>2,000 V</td>
</tr>
<tr>
<td>Focus voltage</td>
<td>725 V</td>
</tr>
<tr>
<td>Sample cone</td>
<td>Standard, Ni</td>
</tr>
<tr>
<td>Skimmer cone</td>
<td>Standard, Ni</td>
</tr>
<tr>
<td>Spray chamber</td>
<td>SIS</td>
</tr>
<tr>
<td>Nebulizer</td>
<td>PFA-ST, 100 μL/min</td>
</tr>
<tr>
<td>Sample uptake rate</td>
<td>65 μL/min</td>
</tr>
<tr>
<td>Uptake mode</td>
<td>Free aspiration</td>
</tr>
<tr>
<td>Instrument Resolution</td>
<td>400 (Low)</td>
</tr>
<tr>
<td>Analyzer pressure mbar</td>
<td>$1 \times 10^{-8}$ mbar</td>
</tr>
<tr>
<td>Minimum sensitivity for $^{88}$Sr (10^{11} Ω resistors)</td>
<td>16 V/ppm</td>
</tr>
<tr>
<td>Blocks</td>
<td>1</td>
</tr>
<tr>
<td>Cycles/block</td>
<td>45</td>
</tr>
<tr>
<td>Integration time</td>
<td>8.41 sec</td>
</tr>
<tr>
<td>Baseline on peak, 2% HNO₃</td>
<td>60 sec</td>
</tr>
</tbody>
</table>

**Cup Configuration**

<table>
<thead>
<tr>
<th>Collection Mode</th>
<th>Static</th>
</tr>
</thead>
<tbody>
<tr>
<td>L3</td>
<td>$^{82}$Kr⁺</td>
</tr>
<tr>
<td>L2</td>
<td>$^{84}$Sr⁺/84Kr⁺</td>
</tr>
<tr>
<td>L1</td>
<td>$^{85}$Rb⁺</td>
</tr>
<tr>
<td>C</td>
<td>$^{86}$Sr⁺/86Kr⁺</td>
</tr>
<tr>
<td>H1</td>
<td>$^{87}$Sr⁺/87Rb⁺</td>
</tr>
<tr>
<td>H2</td>
<td>$^{88}$Sr⁺</td>
</tr>
</tbody>
</table>
The concentration of the NIST 987 Sr standard (100–500 ppb) was varied to assess the effect of signal strength (monitored by $^{88}$Sr) on accuracy and precision (Figure 7). When instrument parameters remained constant and only the solution concentration varied, a clear decrease in measurement precision and a deviation in the accuracy of the measurement were observed with the 100 ppb solution (run at approximately 1 V $^{88}$Sr). This result is consistent with a previous study that showed similar deviation in the accuracy with low signal strength during MC-ICP-MS analysis (Neptune) (De Muynck et al., 2009).

Overall, these results suggest that in order to achieve accurate and precise Sr isotope ratio measurements with the Neptune MC-ICPMS, the $^{88}$Sr signal should be $\geq 8$ V (and $< 50$ V with $10^{11}$ $\Omega$ resistors). This can be achieved with 400 to 500 ppb Sr solutions using standard operating procedures. Optimal tuning of the instrument usually produces a higher $^{88}$Sr signal strength (~15 to 30 volts). This indicates that solutions taken directly from the Sr separation protocol described here, even if Sr yields are as low as 50%, have adequate concentrations of Sr to achieve good accuracy and precision.
Similar tests of accuracy and precision of the NIST 987 Sr standard were conducted using various data acquisition methods (e.g. varied signal integration time, number of sampling blocks, and number of cycles per block). The ideal balance between precision and sample throughput occurred with signal integration times of ~8 sec and 1 block of 45 measurements (or cycles per block). Table 2 describes the optimal instrument parameters for the Neptune MC-ICPMS based on these experiments.

To assess long term variability of the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio, the NIST 987 Sr standard was analyzed over the course of a month using the instrument parameters shown in Table 2 (Figure 8). The average $^{87}\text{Sr}/^{86}\text{Sr}$ value (n=99) is $0.710265 \pm 14 (2\sigma)$. These values are consistent with other measurements of NIST 987 by MC-ICP-MS (De Muynck et al., 2009; Rich et al., 2012).

![Figure 8: $^{87}\text{Sr}/^{86}\text{Sr}$ values of repeat measurement of NIST 987 over 2 weeks. The average value is $0.710265 \pm 14 (2\sigma)$.](image-url)
5. COMPARISON OF MC-ICP-MS AND THERMAL IONIZATION MASS SPECTROMETRY

For comparison of Sr isotope results with standard TIMS analysis of samples, the method described here was used to chemically separate and analyze by MC-ICP-MS samples that were previously measured using a multidynamic method on a Finnigan-MAT 262 thermal ionization mass spectrometer (Table 1). Details of sample preparation and analysis of those samples are discussed elsewhere (Brubaker et al., 2013; Chapman et al., 2012; Chapman et al., 2013; Sharma et al., 2013).

Sr isotope measurements performed by MC-ICP-MS were compared to TIMS on a variety of samples with a wide range of \(^{87}\text{Sr}/^{86}\text{Sr}\) (Table 1). All of these samples had been previously processed through gravity-fed Sr-Resin® columns and analyzed by TIMS (Brubaker et al., 2013; Chapman et al., 2012; Chapman et al., 2013; Sharma et al., 2013). Unseparated aliquots of the same samples were obtained and processed through the entire chemical separation and MC-ICP-MS procedure described in this paper. Even when measured by TIMS, the \(^{87}\text{Sr}/^{86}\text{Sr}\) ratio of the NIST SRM 987 standard on different instruments can vary significantly, depending on the instrument geometry and measurement algorithm. The measured value of this standard is routinely reported to allow inter-laboratory comparison of \(^{87}\text{Sr}/^{86}\text{Sr}\) ratios. Therefore, all measured ratios were normalized to a common value of 0.710240 for the NIST SRM 987 standard by applying the offset between the standard measurements and this value to all measured ratios. To assess the agreement of the \(^{87}\text{Sr}/^{86}\text{Sr}\) ratios measured by TIMS and MC-ICP-MS, a Bland-Altman plot (Figure 8) was used (Bland and Altman, 1986). The average difference of the \(^{87}\text{Sr}/^{86}\text{Sr}\) ratios measured by TIMS and MC-ICP-MS is 1.7x10\(^{-6}\). While this indicates that, for the ten samples that were measured, \(^{87}\text{Sr}/^{86}\text{Sr}\) ratios were measured to be slightly higher using TIMS, this value is smaller than the average standard error of sample measurements by TIMS (8.0x10\(^{-6}\)). Therefore, this can conclude that any bias related to the average difference \(^{87}\text{Sr}/^{86}\text{Sr}\) ratios measured by TIMS and MC-ICP-MS is within the error of the measurement. Furthermore, difference between \(^{87}\text{Sr}/^{86}\text{Sr}\) ratios measured TIMS and MC-ICP-MS is no greater than 1.8x10\(^{-5}\) as indicated by the 95% confidence levels (2\(\sigma\), dark dashes) in Figure 9. This variability is close to the long term precision (2\(\sigma\)) of standard measurements by TIMS (1.7x10\(^{-5}\)). These results suggest that Sr isotopic measurements with a precision and accuracy comparable to routine measurements made by TIMS are achievable using this method.
Figure 9: Differences in $^{87}\text{Sr}/^{86}\text{Sr}$ values measured by the University of Pittsburgh TIMS and MC-ICP-MS vs. the average $^{87}\text{Sr}/^{86}\text{Sr}$ values normalized to a common value for SRM 987 of 0.710240. The error bars represent the propagated error of both measurements. The bold dashed line represents the 2σ error (±0.000018, n = 10) and the light dashed line is the average difference of the $^{87}\text{Sr}/^{86}\text{Sr}$ values (1.7x10⁻⁶).
6. DATA HANDLING AND REDUCTION

6.1 INSTRUMENTAL MASS BIAS CORRECTIONS

Data acquisition was carried out using 1 block of 45 measurements with 8-s integration times. Raw data (voltages) were first corrected for signal contributions using voltages from the analytical blank (2% HNO$_3$). The $^{87}$Sr/$^{86}$Sr ratio was corrected for instrumental mass discrimination using an exponential law (Russell et al., 1978; Wasserburg et al., 1981) assuming a normal $^{86}$Sr/$^{88}$Sr ratio of 0.1194 (De Laeter et al., 2003). The $^{87}$Sr$^+$ signal was corrected for any contribution from $^{87}$Rb$^+$ by measuring $^{85}$Rb$^+$ and assuming a $^{87}$Rb/$^{85}$Rb ratio of 0.3858 (De Laeter et al., 2003). Additionally, the $^{86}$Sr$^+$ signal was corrected to account for any $^{86}$Kr$^+$ contamination present with the Ar source by measuring $^{83}$Kr$^+$ and using a value of 1.5044 for the $^{86}$Kr/$^{83}$Kr ratio (De Laeter et al., 2003). Calcium argide and dimer corrections were not carried out because these interferences have not been observed with the Neptune MC-ICP-MS (Ramos et al., 2004; Yang et al., 2012). After all corrections were applied, any of the 45 measured ratios that fell outside of the 95% ($2\sigma$) confidence test were edited out as outliers. Typically fewer than 3 ratios were removed.

6.2 DATA REDUCTION AND QUALITY ASSURANCE

Since these methods allow for high sample throughput resulting in a potential completion of ~120 samples per day, data management is important. The data output from the Thermo Scientific Neptune software can be cumbersome however, especially when dealing with multiple samples. It is important to not only collect the $^{87}$Sr/$^{86}$Sr ratio, but also monitor other quality assurance parameters such as the $^{88}$Sr signal intensity, the $^{88}$Sr signal from the blank, the magnitude of the Rb and Kr interference correction, and the stability of the measured signals over time. To do this however, the data must be organized by the user. Microsoft Excel macros have been developed that reduce the data to a final user friendly output that appears in Appendix A. This output displays sample information, the isotope ratios, signal intensities, measurement errors, and signal variability over time. An important feature of the data output highlights the normalized $^{87}$Sr/$^{86}$Sr ratio. In order to compare ratios measured across long time periods it is necessary to correct for normal long term instrument drifting. To do this three to five (or more) NIST 978 standard solutions are measured over the course of the run. The average of these standard runs is then compared to 0.710240 and an offset is calculated. This offset is then applied to the $^{87}$Sr/$^{86}$Sr ratio of the sample and the normalized ratio is displayed.

Instructions listed in Appendix B allow data from the entire run to be reduced into easily managed PDF files and a stand-alone Microsoft Excel spreadsheet. The macros are part of files Sr_template.xlsm and appear in Appendix C.
7. **CONCLUSIONS**

A high-throughput Sr separation procedure for $^{87}\text{Sr}/^{86}\text{Sr}$ isotope analysis by MC-ICP-MS was developed, based in part on previously existing vacuum box methods. This procedure is optimized for accurate and precise $^{87}\text{Sr}/^{86}\text{Sr}$ measurements of fluids related oil/gas production and geologic storage of carbon. The chemical separation procedure can effectively isolate Sr from complex sample matrices and from solutions that have excess Ca, K, Ba, and Fe. This separation procedure uses off-the-shelf parts, and is designed with the option to be carried out offsite without the direct need for a dedicated clean lab and mass spectrometry facility. The low cost of the column and resin assembly allows use of a new column and fresh resin for each sample to minimize contamination. This report also describes optimal parameters for MC-ICPMS analysis to achieve routine accuracy with precision of $\pm 1.4 \times 10^{-5}$. After sample evaporation, processing time for 24 samples is approximately 1 hr and a maximum of 120 samples per day can be analyzed using an autosampler by MC-ICP-MS. This is approximately an order of magnitude faster than traditional methods using standard columns combined with TIMS analysis. The results of this high-throughput method demonstrate that Sr isotopes analysis could be a viable tool for MVA and long-term geochemical monitoring of oil/gas reservoirs.
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8. REFERENCES


Hamel, B. L.; Stewart, B. W.; Kim, A. G. Tracing the interaction of acid mine drainage with coal utilization byproducts in a grouted mine: Strontium isotope study of the inactive Omega Coal Mine, West Virginia (USA). Applied Geochemistry 2010, 25, 212–223.


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APPENDIX A: DATA MANAGEMENT EXAMPLE OUTPUT

Neptune Sr Data Reduction

Sample Name: NIST987

Run Date: 3/11/2013
Time: 11:29:33:628
Run number: 002
File: C:\Neptune\User\NEPTUNE\Data\example_folder\NIST987_002.dat
Method Name: C:\Neptune\User\NEPTUNE\Methods\example_folder\120510_ajw_8_3_1_45_Sr.met
Sample ID: NIST987
Operator: ajw
Valid Values: 43(45)

RESULTS

$^{87}\text{Sr}/^{86}\text{Sr}$ normalized to 0.71024: \[0.710245 \pm 1.4\times10^{-5}\] 3SD, see standard results on back

$^{87}\text{Sr}/^{86}\text{Sr}$ as reported NEPTUNE: \[0.710273 \pm 3.5\times10^{-6}\] SE

$^{87}\text{Sr}/^{86}\text{Sr}$ calc, no correction: 0.710797
$^{87}\text{Sr}/^{86}\text{Sr}$ calc, Rb + Kr corr.: 0.710294
$^{87}\text{Sr}/^{86}\text{Sr}$ calc, Rb corr. only: 0.710293

Rb correction: 709.4 ppm
Kr correction: 2.20 ppm

$^{88}\text{Sr}$ (V): 20.06
$^{88}\text{Sr}$ background: 0.004
signal to bkgnd: 5198.

$^{88}\text{Sr}$ max/min (V): 20.2 / 19.6
$^{88}\text{Rb}$ max/min (V): 0.003102 / 0.002992
$^{86}\text{Sr}/^{86}\text{Sr}$ max/min: 0.114676 / 0.114662

Corrected for mass fractionation, Rb, and Kr interference

---

A-1
### Standard Results

(Neptune results, corrected for Rb, Kr, and mass bias)

<table>
<thead>
<tr>
<th>Analysis Date</th>
<th>Time</th>
<th>Sample ID</th>
<th>#</th>
<th>run</th>
<th>87Sr/86Sr</th>
<th>Std Err (ab)</th>
<th>valid values</th>
<th>88Sr</th>
</tr>
</thead>
<tbody>
<tr>
<td>3/11/2013</td>
<td>11:29:33:628</td>
<td>NIST987</td>
<td>2</td>
<td>6</td>
<td>0.710273</td>
<td>3.5E-06</td>
<td>43(45)</td>
<td>20.1</td>
</tr>
<tr>
<td>3/11/2013</td>
<td>11:43:27:628</td>
<td>NIST987</td>
<td>4</td>
<td>6</td>
<td>0.710264</td>
<td>4.4E-06</td>
<td>45(45)</td>
<td>20.0</td>
</tr>
<tr>
<td>3/11/2013</td>
<td>14:16:21:621</td>
<td>NIST987</td>
<td>26</td>
<td>6</td>
<td>0.710278</td>
<td>3.6E-06</td>
<td>44(45)</td>
<td>20.1</td>
</tr>
<tr>
<td>3/11/2013</td>
<td>16:49:12:615</td>
<td>NIST987</td>
<td>48</td>
<td>6</td>
<td>0.710262</td>
<td>3.8E-06</td>
<td>42(45)</td>
<td>20.0</td>
</tr>
<tr>
<td>3/11/2013</td>
<td>17:58:41:611</td>
<td>NIST987</td>
<td>58</td>
<td>6</td>
<td>0.710263</td>
<td>3.6E-06</td>
<td>44(45)</td>
<td>19.8</td>
</tr>
</tbody>
</table>

**Avg Standard**: 0.710268  
**2 Stdev Stneds**: 1.4E-05  
**offset from (0.710240)**: -2.82E-05

#### 88Sr background over entire analytical run

[Graph showing 88Sr background over entire analytical run]
APPENDIX B: SR ISOPIPE DATA REDUCTION FOR THERMO NEPTUNE
The NEPTUNE software creates a folder in which it saves .DAT, .EXP, .TDT, and .LOG files of your analytical run. The .DAT files contain the raw signals from each faraday cup and calculations for any ratios or mass bias corrections that have been selected. These files can be opened by NEPTUNE software (EVALUATION) and are used for reprocessing of the data if adjustments to any ratio calculation are needed. The .LOG files can be read in a text editor and they record some of the instrument conditions from the run. The .EXP files are simply .DAT files that can be read by EXCEL.

To reduce Sr isotope data from the NEPTUNE output files (.EXP) follow this procedure:

1) Open the folder containing your data and verify that there are .EXP files

2) Open Sr_data_reduction folder on the desktop, select “Sr_template.xlsm”, copy, and paste a copy of the template into your data folder (a copy of Sr_template is located in the copy folder in case the original files in corrupted)

3) Close Sr_data_reduction folder

4) Change .exp files to .xls files as follows:
   a. Click “start” menu on the Windows desktop
   b. Select “run” program
   c. Type “cmd” and then OK (this opens Windows command prompt)
   d. Type “cd” then SPACE and without hitting return go to the next step
   e. Select the address from your open data folder and COPY
   f. PASTE into command prompt by right clicking and selected PASTE
   g. Hit RETURN
   h. Type “ren<SPACE> *.exp<SPACE> *.xls” (note the spaces)
   i. Hit RETURN
   j. Go back to your data folder and verify that the .EXP files are now .XLS files
   k. Close command prompt

5) Open EXCEL from the “start” menu

6) On the “Data” tab click “RDBMerge Add-in” to compile all the .XLS files into one
   a. Folder Location → click Browse and navigate to your folder, click OK
   b. Which Files → pull down “XLS”, default: select “Merge All files from the folder…”
   c. Which worksheet(s) → default: “Use the sheet index 1”
   d. Which range → change to First cell A1
   e. Check Add file name, Check Paste as values
   f. Click “MERGE”
   g. Once it is finished click OK
h. Close Book1 without saving

7) In the new spreadsheet, SELECT ALL (Ctrl + A) and COPY all the data in the “Combine Sheet” worksheet

8) Open the copy of “Sr_template.xlsm” from your data folder

9) PASTE the copied data into “Combine Sheet”

10) To start the data processing, Click the blue, red, and yellow circle at the top of the spreadsheet (next to the save button).

11) Once processing is done (~1 min), navigate to print menu, select PRINT, and select the “Adobe PDF” printer, printing “Active sheets”

12) A “save as” prompt will appear, name your file and save it to the desired location

13) PDF will be generated giving a report for each sample. This can be printed using two sided printing so each sample will have a standard summary on the back.

14) IMPORTANT: Save the Sr_template.xlsm of your newly compiled data by SAVE AS, select file type *.xlsx, rename the file and save it to the desired location. Click SAVE, then click YES to save as a macro-free workbook.

15) CLOSE the workbook called Sheet 1 without saving (the file that was created using RDBMerge)

16) Delete the Sr_template.xlsm from your data folder (this prevents having multiple templates scatter across the computer)

The compiled spreadsheet has a tab marked Samples and Standards (scroll all the way to the left). These summarize the data in the order in which they were run and applies the normalization to 0.71024.
APPENDIX C: EXCEL MACRO

Sub main()
Call standardMove
Call cleanupStandards
Call sampleMove
Call cleanupSamples
Call assembleSamples
Call assembleStandards
Call removeEmpty
Call SortSheets
Call activateSheets
'Call printToPDF
End Sub

Sub standardMove()
Const sampletype1 = "SampleType: STD"
Dim wsSource As Worksheet
Dim wsDest As Worksheet
Dim NoRows As Long
Dim DestNoRows As Long
Dim i As Long
Dim rngCells As Range
Dim rngFind As Range
Set wsSource = Worksheets("Combine sheet")
NoRows = wsSource.Range("A65536").End(xlUp).Row
DestNoRows = 5
Set wsDest = ActiveWorkbook.Worksheets.Add
For i = 1 To NoRows
    Set rngCells = wsSource.Range("B" & i)
    '84
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 4).Copy wsDest.Range("q" & DestNoRows)
    End If
    '86
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 6).Copy wsDest.Range("p" & DestNoRows)
    End If
    '87
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 7).Copy wsDest.Range("o" & DestNoRows)
    End If
    '82
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 2).Copy wsDest.Range("n" & DestNoRows)
    End If
    '83
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 3).Copy wsDest.Range("m" & DestNoRows)
    End If
    '85
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 5).Copy wsDest.Range("l" & DestNoRows)
    End If
    'background
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(50, 8).Copy wsDest.Range("j" & DestNoRows)
    End If
    '88
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(51, 8).Copy wsDest.Range("i" & DestNoRows)
    End If
'valid values
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(56, 10).Copy wsDest.Range("h" & DestNoRows)
End If
'standard error (ab)
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(53, 10).Copy wsDest.Range("g" & DestNoRows)
End If
'87/86
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(51, 10).Copy wsDest.Range("f" & DestNoRows)
End If
'run number
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(-8, 0).Copy wsDest.Range("e" & DestNoRows)
End If
'sample id
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(-11, 0).Copy wsDest.Range("d" & DestNoRows)
End If
'time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(47, 1).Copy wsDest.Range("c" & DestNoRows)
End If
'date
If Not (rngCells.Find(sampletype1) Is Nothing) Then
   rngCells.Offset(-5, 0).Copy wsDest.Range("b" & DestNoRows)
End If

DestNoRows = DestNoRows + 1
End If

Next i

ActiveSheet.Name = "Standards"
End Sub

Sub cleanupStandards()
'add headers
   Worksheets("Standards").Range("b4") = "Analysis Date"
   Worksheets("Standards").Range("c4") = "Time"
   Worksheets("Standards").Range("d4") = "Sample ID"
   Worksheets("Standards").Range("e4") = "Run Number"
   Worksheets("Standards").Range("f4") = "87Sr/86Sr"
   Worksheets("Standards").Range("g4") = "Std Err (ab)"
   Worksheets("Standards").Range("h4") = "Valid Values"
   Worksheets("Standards").Range("i4") = "88Sr"
   Worksheets("Standards").Range("j4") = "88Sr bckgrnd"
   Worksheets("Standards").Range("k4") = "85Rb"
   Worksheets("Standards").Range("l4") = "83Kr"
   Worksheets("Standards").Range("m4") = "82Kr"
   Worksheets("Standards").Range("n4") = "87Sr"
   Worksheets("Standards").Range("o4") = "87Sr"
   Worksheets("Standards").Range("p4") = "86Sr"
   Worksheets("Standards").Range("q4") = "84Sr"
   Worksheets("Standards").Range("r4") = "Avg Standard"
   Worksheets("Standards").Range("s4") = "2 Stdev Stnds"
   Worksheets("Standards").Range("t4") = "offset from (0.710240)"

'a1
   Range("a1").Select
   With Selection
      .HorizontalAlignment = xlLeft
   End With
   Worksheets("Standards").Range("a1") = "NEPTUNE Sr Isotope Data: Standards"
   Range("a1").EntireRow.Font.Bold = True

'bold
   Range("A4").EntireRow.Font.Bold = True
'average standards
   Range("S5").Select
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

ActiveCell.FormulaR1C1 = "=AVERAGE(RC[-13]:R[1000]C[-13])"

' 2 Stdev of standards
Range("t5").Select
ActiveCell.FormulaR1C1 = "=2*STDEV(RC[-14]:R[1000]C[-14])"

' offset
Range("u5").Select
ActiveCell.FormulaR1C1 = "=0.71024-RC[-2]"

' remove Analysis date:
Columns("B:B").Select
Selection.Replace What:="Analysis date:", Replacement:="", LookAt:=xlPart, _
SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
ReplaceFormat:=False

' remove Sample ID:
Columns("D:D").Select
Selection.Replace What:="Sample ID:", Replacement:="", LookAt:=xlPart, _
SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
ReplaceFormat:=False

' remove Run number:
Columns("E:E").Select
Selection.Replace What:="Run number:", Replacement:="", LookAt:=xlPart, _
SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
ReplaceFormat:=False

' center text
Cells.Select
With Selection
  .HorizontalAlignment = xlCenter
  .VerticalAlignment = xlBottom
  .WrapText = False
  .Orientation = 0
  .AddIndent = False
  .IndentLevel = 0
  .ShrinkToFit = False
  .ReadingOrder = xlContext
  .MergeCells = False
End With

' format
Columns("F:F").Select
Selection.NumberFormat = "0.000000"
Columns("G:G").Select
Selection.NumberFormat = "0.0E+00"
Columns("I:I").Select
Selection.NumberFormat = "0.0"
Columns("J:J").Select
Selection.NumberFormat = "0.0000"
Columns("L:L").Select
Selection.NumberFormat = "0.0E+00"
Columns("O:O").Select
Selection.NumberFormat = "0.00"
Columns("S:S").Select
Selection.NumberFormat = "0.000000"
Columns("T:T").Select
Selection.NumberFormat = "0.0E+00"
Columns("U:U").Select
Selection.NumberFormat = "0.0E+00"

Cells.Select
Selection.Columns.AutoFit

'sort
Cells.Select
ActiveWorkbook.Worksheets("Standards").Sort.SortFields.Add Key:=Range("E5:E1000"). _
SortOn:=xlSortOnValues, Order:=xlAscending, DataOption:=xlSortNormal
With ActiveWorkbook.Worksheets("Standards").Sort
  .SetRange Range("B4:U1000")
  .Header = xlYes
  .MatchCase = False
  .Orientation = xlTopToBottom
  .SortMethod = x1PinYin
  .Apply
End With
Sub sampleMove()
Const sampletype1 = "SampleType: SMP"
Dim wsSource As Worksheet
Dim wsDest As Worksheet
Dim NoRows As Long
Dim DestNoRows As Long
Dim i As Long
Dim rngCells As Range
Dim rngFind As Range
Set wsSource = Worksheets("Combine sheet")
NoRows = wsSource.Range("A65536").End(xlUp).Row
DestNoRows = 5
Set wsDest = ActiveWorkbook.Worksheets.Add
For i = 1 To NoRows
    Set rngCells = wsSource.Range("B" & i)
    '84
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 4).Copy wsDest.Range("s" & DestNoRows)
    End If
    '86
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 6).Copy wsDest.Range("r" & DestNoRows)
    End If
    '87
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 7).Copy wsDest.Range("q" & DestNoRows)
    End If
    '82
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 2).Copy wsDest.Range("p" & DestNoRows)
    End If
    '83
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 3).Copy wsDest.Range("o" & DestNoRows)
    End If
    '85
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 5).Copy wsDest.Range("n" & DestNoRows)
    End If
    'background
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(50, 8).Copy wsDest.Range("l" & DestNoRows)
    End If
    '88
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 8).Copy wsDest.Range("k" & DestNoRows)
    End If
    'valid values
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(57, 10).Copy wsDest.Range("j" & DestNoRows)
    End If
    'standard error (ab)
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(54, 10).Copy wsDest.Range("i" & DestNoRows)
    End If
    '87/86
    If Not (rngCells.Find(sampletype1) Is Nothing) Then
        rngCells.Offset(52, 10).Copy wsDest.Range("h" & DestNoRows)
    End If
    'run number
    If Not (rngCells.Find(sampletype1) Is Nothing) Then

rngCells.Offset(-8, 0).Copy wsDest.Range("e" & DestNoRows)
End If
'sample id
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(-11, 0).Copy wsDest.Range("d" & DestNoRows)
End If
'time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(47, 1).Copy wsDest.Range("c" & DestNoRows)
End If
'date
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(-5, 0).Copy wsDest.Range("b" & DestNoRows)
End If
DestNoRows = DestNoRows + 1
End If
Next i
ActiveSheet.Name = "Samples"
End Sub

Sub cleanupSamples()
'add headers
Worksheets("Samples").Range("b4") = "Analysis Date"
Worksheets("Samples").Range("c4") = "Time"
Worksheets("Samples").Range("d4") = "Sample ID"
Worksheets("Samples").Range("e4") = "Run Number"
Worksheets("Samples").Range("f4") = "87Sr/86Sr normalized"
Worksheets("Samples").Range("g4") = "2SD standards"
Worksheets("Samples").Range("h4") = "87Sr/86Sr"
Worksheets("Samples").Range("i4") = "Std Err (ab)"
Worksheets("Samples").Range("j4") = "Valid Values"
Worksheets("Samples").Range("k4") = "88Sr"
Worksheets("Samples").Range("l4") = "88Sr backgrnd"
Worksheets("Samples").Range("m4") = "85Rb"
Worksheets("Samples").Range("n4") = "83Kr"
Worksheets("Samples").Range("o4") = "82Kr"
Worksheets("Samples").Range("p4") = "87Sr"
Worksheets("Samples").Range("q4") = "86Sr"
Worksheets("Samples").Range("r4") = "84Sr"

'"a1
Range("a1").Select
With Selection
    .HorizontalAlignment = xlLeft
End With
Worksheets("Samples").Range("a1") = "NEPTUNE Sr Isotope Data: Samples"
Range("a1").EntireRow.Font.Bold = True
'bold
Range("A1").EntireRow.Font.Bold = True
'remove Analysis date:
Columns("B:B").Select
  Selection.Replace What:="Analysis date:", Replacement:="", LookAt:=xlPart _
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
    ReplaceFormat:=False
'remove Sample ID:
Columns("D:D").Select
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
    ReplaceFormat:=False
'remove Run number:
Columns("E:E").Select
  Selection.Replace What:="Run number:", Replacement:="", LookAt:=xlPart _
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
    ReplaceFormat:=False
'center text
Cells.Select
With Selection
    .HorizontalAlignment = xlCenter
    .VerticalAlignment = xlBottom
    .WrapText = False
    .Orientation = 0
    .AddIndent = False
    .IndentLevel = 0
    .ShrinkToFit = False
    .ReadingOrder = xlContext
    .MergeCells = False
End With
'Sort
Cells.Select
ActiveWorkbook.Worksheets("Samples").Sort.SortFields.Clear
With ActiveWorkbook.Worksheets("Samples").Sort
    .SetRange Range("B4:U1000")
    .Header = xlYes
    .MatchCase = False
    .Orientation = xlTopToBottom
    .SortMethod = xlPinYin
    .Apply
End With

'Normalized ratio
Range("F5").Select
Range("F5").Select
Selection.AutoFill Destination:=Range("F5:F500"), Type:=xlFillDefault
Range("F5:F182").Select

'Inserts 2SD standards
Range("G5").Select
ActiveCell.FormulaR1C1 = "=IF(RC[1]>0,Standards!R5C20,)"
Range("G5").Select
Selection.Copy
Range("G5:G500").Select
Selection.Replace What:="0", Replacement:="", LookAt:=xlWhole,
SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False,
ReplaceFormat:=False

Range("A1").Select
End Sub

Sub assembleSamples()
Const samplertype1 = "SampleType: SMP"

C-6
Dim wsSource As Worksheet
Dim wsDest As Worksheet
Dim NoRows As Long
Dim DestNoRows As Long
Dim i As Long
Dim rngCells As Range
Dim rngFind As Range

Set wsSource = Worksheets("Combine sheet")
NoRows = wsSource.Range("A65536").End(xlUp).Row
DestNoRows = 5
Set wsDest = ActiveWorkbook.Worksheets.Add

For i = 1 To NoRows
    Set rngCells = wsSource.Range("B" & i)

'sample id
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-11, 0).Copy wsDest.Range("c" & 2)
    'remove Sample ID:
    Columns("c:c").Select
    Selection.Replace What:="Sample ID:", Replacement:="", LookAt:=xlPart
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, ReplaceFormat:=False
End If
'date
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-5, 0).Copy wsDest.Range("b" & 4)
    'remove Analysis date:
    Columns("b:b").Select
    Selection.Replace What:="Analysis date:", Replacement:="", LookAt:=xlPart
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, ReplaceFormat:=False
End If
'time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(47, 1).Copy wsDest.Range("b" & 5)
End If
'run number
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-8, 0).Copy wsDest.Range("b" & 6)
    'remove Run number:
    Columns("b:b").Select
    Selection.Replace What:="Run number:", Replacement:="", LookAt:=xlPart
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, ReplaceFormat:=False
End If
'file location
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-13, 0).Copy wsDest.Range("b" & 7)
    'remove file location:
    Columns("b:b").Select
    Selection.Replace What:="Filename:", Replacement:="", LookAt:=xlPart
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, ReplaceFormat:=False
End If
'method name
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-10, 0).Copy wsDest.Range("b" & 8)
    'remove method name:
    Columns("b:b").Select
    Selection.Replace What:="Method Name:", Replacement:="", LookAt:=xlPart
    , SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, ReplaceFormat:=False
End If
'sample id
If Not (rngCells.Find(sampletype1) Is Nothing) Then
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, ReplaceFormat:=False
\n'entire sample set, run number
Rang("R6").Select
ActiveCell.FormulaR1C1 = "=Samples!R[-1]C[-6]"
Rang("R6").Select
Selection.AutoFill Destination:=Range("R6:R500"), Type:=xlFillDefault
Rang("R6:R500").Select
Selection.Copy
End If
'84
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 4).Copy wsDest.Range("o" & 2)
End If
'86
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 6).Copy wsDest.Range("n" & 2)
End If
'87
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 7).Copy wsDest.Range("m" & 2)
End If
'82
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 2).Copy wsDest.Range("l" & 2)
End If
'83
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 3).Copy wsDest.Range("k" & 2)
End If
'85
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 5).Copy wsDest.Range("j" & 2)
End If
'87/86
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 10).Copy wsDest.Range("c" & 13)
End If
'standard error (ab)
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(54, 10).Copy wsDest.Range("e" & 13)
End If
'calculations
'Standard normalization
Range("C11").Select
Range("E11").Select
'pull 2SD of Standard measurement
ActiveCell.FormulaR1C1 = "=Standards!R[-6]C[15]"
Range("E12").Select
End If
'88
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(52, 8).Copy wsDest.Range("b" & 19)
End If
'background
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(50, 8).Copy wsDest.Range("b" & 20)
End If
'87/86 calc, no correction
Range("C15").Select
87Sr Rb corr.
Range("P2").Select
ActiveCell.FormulaR1C1 = "=(R[-13]C[-3]-(RC[-6]*(0.3857563))" Range("P2").Select
86Sr Kr corr.
Range("Q2").Select
ActiveCell.FormulaR1C1 = "=(R[-13]C[-3]-(RC[-6]*(1.50434765))" Range("Q2").Select
'87/86 calc, Rb+Kr corr:
Range("C16").Select
'87/86 calc, Rb only corr:
Range("C17").Select
'87/86 calc, Rb only corr:
Range("C17").Select
'87/86 calc, Rb+Kr corr:
Range("P2").Select
87Sr Rb corr.
Range("Q2").Select
ActiveCell.FormulaR1C1 = "=(R[-13]C[-3]-(RC[-6]*(0.3857563))" Range("Q2").Select
86Sr Kr corr.
Range("C16").Select
'87/86 calc, Rb only corr:
Range("C17").Select
'87/86 calc, Rb+Kr corr:
Range("P2").Select
87Sr Rb corr.
Range("Q2").Select
ActiveCell.FormulaR1C1 = "=(R[-13]C[-3]-(RC[-6]*(0.3857563))" Range("Q2").Select
86Sr Kr corr.
Range("C16").Select
'87/86 calc, Rb only corr:
Range("C17").Select
'87/86 calc, Rb+Kr corr:
Range("P2").Select
87Sr Rb corr.
Range("Q2").Select
ActiveCell.FormulaR1C1 = "=(R[-13]C[-3]-(RC[-6]*(0.3857563))" Range("Q2").Select
86Sr Kr corr.
Range("C16").Select
'87/86 calc, Rb only corr:
Range("G15").Select
ActiveCell.FormulaR1C1 = "=(ABS(R[2]C[-4]-RC[-4])/RC[-4]*1000000)" Range("G15").Select
'Rb correction ppm
Range("G16").Select
'Kr correction ppm
Range("B21").Select
ActiveCell.FormulaR1C1 = "=-R[-2]C/R[-1]C" Range("B21").Select
'88 max
Range("F19").Select
ActiveCell.FormulaR1C1 = "=MAX(R[-13]C[6]:R[31]C[6])" Range("F19").Select
'88 min
Range("h19").Select
ActiveCell.FormulaR1C1 = "=MIN(R[-13]C[4]:R[31]C[4])" Range("h19").Select
'85 max
Range("F20").Select
ActiveCell.FormulaR1C1 = "=MAX(R[-14]C[9]:R[30]C[9])" Range("F20").Select
'85 min
Range("h20").Select
ActiveCell.FormulaR1C1 = "=MIN(R[-14]C[7]:R[30]C[7])" Range("h20").Select
'86/88 max
Range("F21").Select
ActiveCell.FormulaR1C1 = "=MAX(R[-15]C[8]:R[29]C[8])" Range("F21").Select
'86/88 min
Range("h21").Select
ActiveCell.FormulaR1C1 = "=MIN(R[-15]C[6]:R[29]C[6])" Range("h21").Select
'87/86 ave plot left
Range("k51").Select
ActiveCell.FormulaR1C1 = "=Average(R[-45]C:R[-1]C)" Range("k51").Select
'87/86 ave plot right
Range("k52").Select
ActiveCell.FormulaR1C1 = "=Average(R[-46]C:R[-2]C)" Range("k52").Select
'87/86 2sd left
Range("k53").Select
ActiveCell.FormulaR1C1 = "=-2*STDEV(R[-47]C:R[-3]C)+R[-2]C" Range("k53").Select
'87/86 2sd right
Columns("m:m").Select
Columns("n:n").Select
Columns("o:o").Select
Columns("p:p").Select
Columns("q:q").Select
Columns("r:r").Select
Rows("1:1").Select
Rows("2:2").Select
Rows("3:3").Select
Rows("4:4").Select
Rows("11:11").Select
Rows("13:13").Select
Rows("22:22").Select

'add headers and lines
Cells.Select
With Selection
  .HorizontalAlignment = xlCenter
End With
'TOP
  'a1
  ActiveSheet.Range("a1") = "Neptune Sr Data Reduction"
  Range("a1").Select
  With Selection.Font
    .FontStyle = "Bold"
    .Size = 12
  End With
  With Selection
    .HorizontalAlignment = xlLeft
  End With
  'a2
  ActiveSheet.Range("a2") = "Sample Name:"
  Range("a2").Select
  With Selection.Font
    .FontStyle = "Italic"
  End With
  With Selection
    .HorizontalAlignment = xlRight
  End With
  'b2 underline
  Range("B2:G2").Select
  With Selection.Borders(xlEdgeBottom)
    .LineStyle = xlContinuous
    .Weight = xlThin
  End With
  'c2
  Range("c2").Select
  With Selection.Font
    .FontStyle = "Bold"
    .Size = 12
  End With
  'd4
  ActiveSheet.Range("a4") = "Run Date:"
  Range("a4").Select
  With Selection.Font
    .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
' b4 underline
Range("B4").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With

ActiveSheet.Range("a5") = "Time:"
Range("a5").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
' b5 underline
Range("B5").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With

ActiveSheet.Range("a6") = "Run number:"
Range("a6").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
' b6 underline
Range("B6").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
' c4
ActiveSheet.Range("c4") = "Sample ID:"
Range("c4").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
' f4 underline
Range("f4").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
' e5
ActiveSheet.Range("e5") = "Operator:"
Range("e5").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
' f5 underline
Range("f5").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

ActiveSheet.Range("e6") = "Valid Values:"
Range("e6").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'S6 underline
Range("f6").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'S7
ActiveSheet.Range("a7") = "File:"
Range("a7").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'a8
ActiveSheet.Range("a8") = "Method Name:"
Range("a8").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'b7
Range("b7").Select
With Selection.Font
  .Size = 8
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
'b8
Range("b8").Select
With Selection.Font
  .Size = 8
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
'a9:a9 underline
Range("a9:i9").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlMedium
End With
'RESULTS
'a10
ActiveSheet.Range("a10") = "RESULTS"
Range("a10").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
'b11
ActiveSheet.Range("b11") = "87Sr/86Sr normalized to 0.71024:"
Range("b11").Select
With Selection.Font
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

..Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
..Superscript = False
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
..Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
..Superscript = False
End With
'c13
Range("c13").Select
Selection.NumberFormat = "0.000000"
'd13
ActiveSheet.Range("d13") = "\"\nRange("d13").Select
'c13
Range("e13").Select
Selection.NumberFormat = "0.0E+00"
'f13
ActiveSheet.Range("f13") = "SE"
Range("f13").Select
With Selection
..HorizontalAlignment = xlLeft
End With
'c13 underline
Range("c13:e13").Select
With Selection.Borders(xlEdgeBottom)
..LineStyle = xlContinuous
..Weight = xlThin
End With
'b15
ActiveSheet.Range("b15") = "87Sr/86Sr calc, no correction:"
Range("b15").Select
With Selection.Font
..FontStyle = "Italic"
..Size = 11
End With
With Selection
..HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
..Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
..Superscript = False
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
..Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
..Superscript = False
End With
'c15 number and underline
Range("c15").Select
Selection.NumberFormat = "0.000000"
With Selection.Borders(xlEdgeBottom)
..LineStyle = xlContinuous
..Weight = xlThin
End With
'b16
ActiveSheet.Range("b16") = "87Sr/86Sr calc, Rb + Kr corr.:"
Range("b16").Select
With Selection.Font
..FontStyle = "Italic"
..Size = 11
End With
With Selection
..HorizontalAlignment = xlRight
End With

C-16
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
  .Superscript = False
End With
'c16 number and underline
Range("c16").Select
Selection.NumberFormat = "0.000000"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'b17
ActiveSheet.Range("b17") = "87Sr/86Sr calc, Rb corr. only:"
Range("b17").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
  .Superscript = False
End With
'c17 number and underline
Range("c17").Select
Selection.NumberFormat = "0.000000"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'f15
ActiveSheet.Range("f15") = "Rb correction"
Range("f15").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'g15 number and underline
Range("g15").Select
Selection.NumberFormat = "0.0"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'h15
ActiveSheet.Range("h15") = "ppm"
Range("h15").Select
With Selection
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

End With 'a21
ActiveSheet.Range("a21") = "signal to bckgrnd"
Range("a21").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'b21 number and underline
Range("b21").Select
Selection.NumberFormat = "0."
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'c19
ActiveSheet.Range("c19") = "88Sr max/min (V):
"Range("c19").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
'f19 number and underline
Range("f19").Select
Selection.NumberFormat = "0.0"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
Range("f19:h19").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
Range("h19").Select
Selection.NumberFormat = "0.0"
With Selection
  .HorizontalAlignment = xlLeft
End With
ActiveSheet.Range("g19") = ":"
Range("g19").Select
'c20
ActiveSheet.Range("e20") = "88Rb max/min (V):
"Range("e20").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
'f20 number and underline
Range("f20").Select
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

Range("m1").Select
ActiveSheet.Range("m1") = "87Sr"
Range("n1").Select
ActiveSheet.Range("n1") = "86Sr"
Range("o1").Select
ActiveSheet.Range("o1") = "84Sr"
Range("p1").Select
ActiveSheet.Range("p1") = "87Sr Rb corr."
Range("q1").Select
ActiveSheet.Range("q1") = "86Sr Kr corr."
Range("r5").Select
ActiveSheet.Range("r5") = "run number"
Range("s5").Select
ActiveSheet.Range("s5") = "88Sr background"
Range("t5").Select
ActiveSheet.Range("t5") = "88Sr background"
Range("u5").Select
ActiveSheet.Range("u5") = "88Sr background"
Range("v5").Select
ActiveSheet.Range("v5") = "88Sr background"

Range("z5") = "Standard Results"

Range("a50").Select
With Selection.Font
 .FontStyle = "Bold"
 .Size = 11
End With
With Selection
 .HorizontalAlignment = xlLeft
End With

Range("b50") = "(Neptune results, corrected for Rb, Kr, and mass bias)"
Range("b50").Select
With Selection.Font
 .FontStyle = "Bold"
 .Size = 11
End With

Range("c76").Select
With Selection.Font
 .FontStyle = "Bold"
 .Size = 11
End With

Sub assembleStandards()
    Const sampletype1 = "SampleType: STD"
    Dim wsSource As Worksheet
    Dim wsDest As Worksheet
    Dim NoRows As Long
    Dim DestNoRows As Long
    Dim i As Long
    Dim rngCells As Range
    ActiveSheet.PageSetup.PrintArea = "$A$1:$i$93"
    Range("A1").Select
    Rename
    ActiveSheet.Name = Range("f4").Value & " " & Range("b6").Value

    'add new worksheet and loop to top
    Set wsDest = ActiveWorkbook.Worksheets.Add
    DestNoRows = DestNoRows + 1
    Next i

End Sub
```vba
Dim rngFind As Range

Set wsSource = Worksheets("Combine sheet")

NoRows = wsSource.Range("A65536").End(xlUp).Row
DestNoRows = 5
Set wsDest = ActiveWorkbook.Worksheets.Add

For i = 1 To NoRows

Set rngCells = wsSource.Range("B" & i)

'sample id
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-11, 0).Copy wsDest.Range("c" & 2)
    Columns("c:c").Select
End If
'date
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-5, 0).Copy wsDest.Range("b" & 4)
    Columns("b:b").Select
End If
'time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(47, 1).Copy wsDest.Range("b" & 5)
End If
'run number
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-8, 0).Copy wsDest.Range("b" & 6)
    Columns("b:b").Select
End If
'File location
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-13, 0).Copy wsDest.Range("b" & 7)
    Columns("b:b").Select
End If
'method name
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-10, 0).Copy wsDest.Range("b" & 8)
    Columns("b:b").Select
End If
'sample id
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-11, 0).Copy wsDest.Range("f" & 4)
    Columns("f:f").Select
End If
```
End If
'operator
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(-3, 0).Copy wsDest.Range("f" & 5)
'remove operator:
    Columns("f:f").Select
End If
'valid values
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(56, 10).Copy wsDest.Range("f" & 6)
End If

'83Kr over time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(2, 3).Resize(46, 1).Copy wsDest.Range("p" & 5)
End If
'85Rb over time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(2, 5).Resize(46, 1).Copy wsDest.Range("o" & 5)
End If
'88Sr/86Sr over time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(2, 11).Resize(46, 1).Copy wsDest.Range("m" & 5)
End If

'CALC FOR 86/88
Range("N6").Select
ActiveCell.FormulaR1C1 = "+=(RC[-1]>0,1/RC[-1]),"
Range("N6").Select
Selection.AutoFill Destination:=Range("N6:N50"), Type:=xlFillDefault
Range("N6:N50").Select
Selection.Copy
End If

'88Sr over time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(2, 8).Resize(46, 1).Copy wsDest.Range("l" & 5)
End If
'87/86 over time
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(2, 10).Resize(46, 1).Copy wsDest.Range("k" & 5)
End If
'cycle number
If Not (rngCells.Find(sampletype1) Is Nothing) Then
    rngCells.Offset(2, 0).Resize(46, 1).Copy wsDest.Range("j" & 5)
End If

'entire sample set, run number
Range("Q6").Select
ActiveCell.FormulaR1C1 = "+=(Samples!R[-1]C[-12],"
Range("Q6").Select
Selection.AutoFill Destination:=Range("Q6:Q500"), Type:=xlFillDefault
Range("Q6:Q500").Select
Selection.Copy
End If
'entire sample set, run number
Range("R6").Select
ActiveCell.FormulaR1C1 = "+=(Samples!R[-1]C[-6],"
Range("R6").Select
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

Selection.AutoFill Destination:=Range("R6:R500"), Type:=xlFillDefault
Range("R6:R500").Select
Selection.Copy
Selection.PasteSpecial Paste:=xlPasteValues, Operation:=xlNone, SkipBlanks _
:=False, Transpose:=False
Selection.Replace What:="0", Replacement:="", LookAt:=xlWhole, _
SearchOrder:=xlByRows, MatchCase:=False, SearchFormat:=False, _
ReplaceFormat:=False
End If
'84
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 4).Copy wsDest.Range("o" & 2)
End If
'86
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 6).Copy wsDest.Range("n" & 2)
End If
'87
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 7).Copy wsDest.Range("m" & 2)
End If
'82
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 2).Copy wsDest.Range("l" & 2)
End If
'83
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 3).Copy wsDest.Range("k" & 2)
End If
'85
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 5).Copy wsDest.Range("j" & 2)
End If

'87/86
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 10).Copy wsDest.Range("c" & 13)
End If
'Standard error (ab)
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(53, 10).Copy wsDest.Range("e" & 13)
End If
'calculations
'Standard normalization
Range("C11").Select
Range("E11").Select
'pull 2SD of Standard measurement
ActiveCell.FormulaR1C1 = ";=Standards!R[-6]C[15]"
Range("E12").Select
End If
'88
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(51, 8).Copy wsDest.Range("b" & 19)
End If
'background
If Not (rngCells.Find(sampletype1) Is Nothing) Then
rngCells.Offset(50, 8).Copy wsDest.Range("b" & 20)
End If
'calculations
'87/86 calc, no correction
Range("C15").Select
Range("C15").Select
'87Sr Rb corr.
Range("P2").Select
ActiveCell.FormulaR1C1 = ";=RC[-3]-(RC[-6]*(0.3857563))"
Range("R2").Select  
'86Sr Kr corr:  
Ranger("Q2").Select  
ActiveCell.FormulaR1C1 = "+RC[-3]*(RC[-6]*(1.50434756))"  
Ranger("Q2").Select  
'87/86 calc, Rb+Kr corr:  
Ranger("C16").Select  
Ranger("C16").Select  
'87/86 calc, Rb only corr:  
Ranger("C17").Select  
ActiveCell.FormulaR1C1 = "+R[-2]C/R[-1]C"  
Ranger("B21").Select  
'Rb correction ppm  
Ranger("G15").Select  
ActiveCell.FormulaR1C1 = "+ABS(R[2]C[4]-RC[4])*1000000"  
Ranger("G16").Select  
'Kr correction ppm  
Ranger("G15").Select  
ActiveCell.FormulaR1C1 = "+(ABS(R[1]C[4]-R[1]C[-4])*1000000)-(ABS(RC[-4]-R[-4])*1000000)"  
Ranger("B21").Select  
'Signal to Background  
Ranger("C17").Select  
Ranger("B21").Select  
'88 max  
Ranger("F19").Select  
ActiveCell.FormulaR1C1 = "+MAX(R[-13]C[6]:R[31]C[6])"  
Ranger("F19").Select  
'88 min  
Ranger("H19").Select  
ActiveCell.FormulaR1C1 = "+MIN(R[-13]C[4]:R[31]C[4])"  
Ranger("H19").Select  
'85 max  
Ranger("F20").Select  
ActiveCell.FormulaR1C1 = "+MAX(R[-14]C[9]:R[30]C[9])"  
Ranger("F20").Select  
'85 min  
Ranger("H20").Select  
ActiveCell.FormulaR1C1 = "+MIN(R[-14]C[7]:R[30]C[7])"  
Ranger("H20").Select  
'86/88 max  
Ranger("F21").Select  
ActiveCell.FormulaR1C1 = "+MAX(R[-15]C[8]:R[29]C[8])"  
Ranger("F21").Select  
'86/88 min  
Ranger("H21").Select  
ActiveCell.FormulaR1C1 = "+MIN(R[-15]C[6]:R[29]C[6])"  
Ranger("H21").Select  
'87/86 ave plot left  
Ranger("k51").Select  
ActiveCell.FormulaR1C1 = "+Average(R[-45]C:R[-1]C)"  
Ranger("k51").Select  
'87/86 ave plot right  
Ranger("k52").Select  
ActiveCell.FormulaR1C1 = "+Average(R[-46]C:R[-2]C)"  
Ranger("k52").Select  
'87/86 2sd left  
Ranger("k53").Select  
ActiveCell.FormulaR1C1 = "+2*STDEV(R[-47]C:R[-3]C)+R[-2]C"  
Ranger("k53").Select  
'87/86 2sd right  
Ranger("k54").Select  
ActiveCell.FormulaR1C1 = "+2*STDEV(R[-48]C:R[-4]C)+R[-3]C"  
Ranger("k54").Select  
'87/86 2sd left  
Ranger("k55").Select  
Columns("p:p").Select
    Selection.columnWidth = 14
Columns("q:q").Select
    Selection.columnWidth = 14
Columns("r:r").Select
    Selection.columnWidth = 14

Rows("1:1").Select
    Selection.rowHeight = 15.75
Rows("2:2").Select
    Selection.rowHeight = 15.75
Rows("3:3").Select
    Selection.rowHeight = 7.5
Rows("4:4").Select
    Selection.rowHeight = 15.75
Rows("11:11").Select
    Selection.rowHeight = 19
Rows("13:13").Select
    Selection.rowHeight = 17.25
Rows("22:22").Select
    Selection.rowHeight = 8.25

'add headers and lines
Cells.Select
With Selection
    .HorizontalAlignment = xlCenter
End With
'TOP
    'a1
    ActiveSheet.Range("a1") = "Neptune Sr Data Reduction"
    Range("a1").Select
    With Selection.Font
        .FontStyle = "Bold"
        .Size = 12
    End With
End With
With Selection
    .HorizontalAlignment = xlLeft
End With
    'a2
    ActiveSheet.Range("a2") = "Sample Name:"
    Range("a2").Select
    With Selection.Font
        .FontStyle = "Italic"
    End With
End With
With Selection
    .HorizontalAlignment = xlRight
End With
'b2 underline
    Range("B2:G2").Select
    With Selection.Borders(xlEdgeBottom)
        .LineStyle = xlContinuous
        .Weight = xlThin
    End With
End With
'c2
    Range("c2").Select
    With Selection.Font
        .FontStyle = "Bold"
        .Size = 12
    End With
End With
'a4
    ActiveSheet.Range("a4") = "Run Date:"
    Range("a4").Select
    With Selection.Font
        .FontStyle = "Italic"
    End With
End With
With Selection
    .HorizontalAlignment = xlRight
End With
'b4 underline
    Range("B4").Select
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

With Selection.Borders(xlEdgeBottom)
    .LineStyle = xlContinuous
    .Weight = xlThin
End With
'a5
ActiveSheet.Range("a5") = "Time:"
Range("a5").Select
With Selection.Font
    .FontStyle = "Italic"
End With
With Selection
    .HorizontalAlignment = xlRight
End With
'b5 underline
Range("B5").Select
With Selection.Borders(xlEdgeBottom)
    .LineStyle = xlContinuous
    .Weight = xlThin
End With
'a6
ActiveSheet.Range("a6") = "Run number:"
Range("a6").Select
With Selection.Font
    .FontStyle = "Italic"
End With
With Selection
    .HorizontalAlignment = xlRight
End With
'b6 underline
Range("B6").Select
With Selection.Borders(xlEdgeBottom)
    .LineStyle = xlContinuous
    .Weight = xlThin
End With
'c4
ActiveSheet.Range("c4") = "Sample ID:"
Range("c4").Select
With Selection.Font
    .FontStyle = "Italic"
End With
With Selection
    .HorizontalAlignment = xlRight
End With
'c5 underline
Range("c5").Select
With Selection.Borders(xlEdgeBottom)
    .LineStyle = xlContinuous
    .Weight = xlThin
End With
'e4
ActiveSheet.Range("e4") = "Operator:"
Range("e4").Select
With Selection.Font
    .FontStyle = "Italic"
End With
With Selection
    .HorizontalAlignment = xlRight
End With
'e5 underline
Range("e5").Select
With Selection.Borders(xlEdgeBottom)
    .LineStyle = xlContinuous
    .Weight = xlThin
End With
'e6
ActiveSheet.Range("e6") = "Valid Values:"
Range("e6").Select
With Selection.Font
    .FontStyle = "Italic"
End With
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

With Selection
  .HorizontalAlignment = xlRight
End With
'c6 underline
Range("c6").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'a7
ActiveSheet.Range("a7") = "File:"
Range("a7").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'a8
ActiveSheet.Range("a8") = "Method Name:
Range("a8").Select
With Selection.Font
  .FontStyle = "Italic"
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'b7
Range("b7").Select
With Selection.Font
  .Size = 8
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
'b8
Range("b8").Select
With Selection.Font
  .Size = 8
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
'a9:a9 underline
Range("a9:i9").Select
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlMedium
End With
'RESULTS
'a10
ActiveSheet.Range("a10") = "RESULTS"
Range("a10").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
'b11
ActiveSheet.Range("b11") = "87Sr/86Sr normalized to 0.71024:"
Range("b11").Select
With Selection.Font
  .FontStyle = "Bold Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
### High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

<table>
<thead>
<tr>
<th>Box 1</th>
<th>Box 2</th>
<th>Box 3</th>
<th>Box 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>±0.000000</td>
<td>±0.0E+00</td>
<td>±87Sr/86Sr</td>
<td>±87Sr/86Sr as reported NEPTUNE:</td>
</tr>
</tbody>
</table>

87Sr/86Sr as reported NEPTUNE:
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

---

...Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
...Superscript = False
End With
'c13
Range("c13").Select
Selection.NumberFormat = "0.000000"
'd13
ActiveSheet.Range("d13") = "+"
Range("d13").Select
'c13
Range("c13").Select
Selection.NumberFormat = "0.0E+00"
'f13
ActiveSheet.Range("f13") = "SE"
Range("f13").Select
With Selection
...HorizontalAlignment = xlLeft
End With
'c13 underline
Range("c13:e13").Select
With Selection.Borders(xlEdgeBottom)
...LineStyle = xlContinuous
...Weight = xlThin
End With
'b15
ActiveSheet.Range("b15") = "87Sr/86Sr calc, no correction:"
Range("b15").Select
With Selection.Font
...FontStyle = "Italic"
...Size = 11
End With
With Selection
...HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
...Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
...Superscript = False
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
...Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
...Superscript = False
End With
'c15 number and underline
Range("c15").Select
Selection.NumberFormat = "0.000000"
With Selection.Borders(xlEdgeBottom)
...LineStyle = xlContinuous
...Weight = xlThin
End With
'b16
ActiveSheet.Range("b16") = "87Sr/86Sr calc, Rb + Kr corr.:"
Range("b16").Select
With Selection.Font
...FontStyle = "Italic"
...Size = 11
End With
With Selection
...HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
...Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
...Superscript = False
End With

---

C-32
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
  .Superscript = False
End With
'c16 number and underline
Range("c16").Select
Selection.NumberFormat = "0.000000"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'b17
ActiveSheet.Range("b17") = "87Sr/86Sr calc, Rb corr. only:"
Range("b17").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
  .Superscript = True
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
  .Superscript = False
End With
'c17 number and underline
Range("c17").Select
Selection.NumberFormat = "0.000000"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'f15
ActiveSheet.Range("f15") = "Rb correction"
Range("f15").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'g15 number and underline
Range("g15").Select
Selection.NumberFormat = "0.0"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
'h15
ActiveSheet.Range("h15") = "ppm"
Range("h15").Select
With Selection
  .HorizontalAlignment = xlLeft
End With
'f16
ActiveSheet.Range("f16") = "Kr correction"
Range("f16").Select
With Selection.Font
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

.FontStyle = "Italic"
.Size = 11
End With
With Selection
  .HorizontalAlignment = xlRight
End With
'g16 number and underline
Range("g16").Select
Selection.NumberFormat = "0.00"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
End With
'!h16
ActiveSheet.Range("h16") = "ppm"
Range("h16").Select
With Selection
  .HorizontalAlignment = xlLeft
End With
'a19
ActiveSheet.Range("a19") = "\(^{88}\)Sr (V):"
Range("a19").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
'!b19 number and underline
Range("b19").Select
Selection.NumberFormat = "0.00"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
End With
'a20
ActiveSheet.Range("a20") = "\(^{88}\)Sr background:"
Range("a20").Select
With Selection.Font
  .FontStyle = "Italic"
  .Size = 11
End With
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
  .Superscript = True
End With
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
  .Superscript = False
End With
'!b20 number and underline
Range("b20").Select
Selection.NumberFormat = "0.000"
With Selection.Borders(xlEdgeBottom)
  .LineStyle = xlContinuous
  .Weight = xlThin
End With
End With
'a21
ActiveSheet.Range("a21") = "signal to bckgrnd"
Range("a21").Select
With Selection.Font
  .FontStyle = "Italic"
End With
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

...
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

LineStyle = xlContinuous
Weight = xlThin
End With
Range("h20").Select
Selection.NumberFormat = "0.000000"
With Selection
HorizontalAlignment = xlLeft
End With
ActiveSheet.Range("g20") = ","
Range("g20").Select
'c21
ActiveSheet.Range("e21") = "86Sr/88Sr max/min:"
Range("e21").Select
With Selection.Font
.FontStyle = "Italic"
.Size = 11
End With
End With
With ActiveCell.Characters(Start:=1, Length:=2).Font
.Superscript = True
End With
End With
With ActiveCell.Characters(Start:=3, Length:=3).Font
.Superscript = False
End With
End With
With ActiveCell.Characters(Start:=6, Length:=2).Font
.Superscript = True
End With
End With
With ActiveCell.Characters(Start:=8, Length:=3).Font
.Superscript = False
End With
End With
'f21 number and underline
Range("f21").Select
Selection.NumberFormat = "0.000000"
With Selection
.HorizontalAlignment = xlRight
End With
End With
Range("f21:h21").Select
With Selection.Borders(xlEdgeBottom)
.LineStyle = xlContinuous
.Weight = xlThin
End With
End With
Range("h21").Select
Selection.NumberFormat = "0.000000"
With Selection
.HorizontalAlignment = xlLeft
End With
ActiveSheet.Range("g21") = ","
Range("g21").Select
'line
Range("a21:i21").Select
With Selection.Borders(xlEdgeBottom)
.LineStyle = xlContinuous
.Weight = xlMedium
End With
'data labels
ActiveSheet.Range("j1") = "85Rb"
Range("j1").Select
ActiveSheet.Range("k1") = "83Kr"
Range("k1").Select
ActiveSheet.Range("l1") = "82Kr"
Range("l1").Select
ActiveSheet.Range("m1") = "87Sr"
Range("m1").Select
ActiveSheet.Range("n1") = "86Sr"
Range("n1").Select
ActiveSheet.Range("o1") = "84Sr"
High-Throughput Method for Sr Isotope Analysis by MC-ICP-MS

Range("a1").Select
ActiveSheet.Range("p1") = "87Sr Rb corr."
Range("p1").Select
ActiveSheet.Range("q1") = "86Sr Kr corr."
Range("q1").Select
ActiveSheet.Range("n5") = "86/88"  
Range("n5").Select
ActiveSheet.Range("q5") = "run number"
Range("q5").Select
ActiveSheet.Range("r5") = "88Sr background"
Range("r5").Select
ActiveSheet.Range("j51") = "0"
Range("j51").Select
ActiveSheet.Range("j52") = "45"
Range("j52").Select
ActiveSheet.Range("j53") = "0"
Range("j53").Select
ActiveSheet.Range("j54") = "45"
Range("j54").Select
ActiveSheet.Range("j55") = "0"
Range("j55").Select
ActiveSheet.Range("j56") = "45"
Range("j56").Select
ActiveSheet.Range("d51") = "run"
Range("d51").Select
ActiveSheet.Range("d52") = "μμ"  
Range("d52").Select
ActiveSheet.Range("g51") = "valid"
Range("g51").Select
ActiveSheet.Range("g52") = "values"
Range("g52").Select
ActivexSheets.Range("a50") = "Standard Results"  
Range("a50").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
End With
With Selection
  .HorizontalAlignment = xlLeft
End With
ActiveSheet.Range("b50") = "(Neptune results, corrected for Rb, Kr, and mass bias)"
Range("b50").Select
Range("a52:h52").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
Range("a76:c76").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
Range("d51:g51").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
Range("e53:e74").Select
Selection.NumberFormat = "0.000000"
Range("f53:f74").Select
Selection.NumberFormat = "0.0E+00"
Range("h53:h74").Select
Selection.NumberFormat = "0.0"
Range("a77").Select
Selection.NumberFormat = "0.000000"
Range("b77").Select
Selection.NumberFormat = "0.0E+00"
Range("c77").Select
Selection.NumberFormat = "0.00E+00"

ActiveSheet.Range("a79") = "88Sr background over entire analytical run"
Range("a79").Select
With Selection.Font
  .FontStyle = "Bold"
  .Size = 11
End With
With Selection
  .HorizontalAlignment = xlLeft
End With

ActiveSheet.Range("a23") = "Corrected for mass fractionation, Rb, and Kr interference"
Range("a23").Select
With Selection
  .HorizontalAlignment = xlLeft
End With

b6 number format
Range("b6").Select
Selection.NumberFormat = "000."

Call Chart8786
Call ChartSr88V
Call ChartRb85V
Call ChartKr86V
Call ChartBckgrnd
ActiveSheet.PageSetup.PrintArea = "$A$1:$i$93"
Range("A1").Select

rename
ActiveSheet.Name = Range("f4").Value & " " & Range("b6").Value

'add new worksheet and loop to top
  Set wsDest = ActiveWorkbook.Worksheets.Add
  DestNoRows = DestNoRows + 1
End If

Next i
End Sub

Sub removeEmpty()

Dim ws As Worksheet
For Each ws In Worksheets
  If ws.Range("A1").Value = "" Then
    Application.DisplayAlerts = False
    ws.Delete
    Application.DisplayAlerts = True
  End If
Next ws
End Sub
Sub SortSheets()
Dim lCount As Long, lCounted As Long
Dim lShtLast As Long
Dim lReply As Long

lShtLast = Sheets.Count
For lCount = 1 To lShtLast
    For lCount2 = lCount To lShtLast
        If UCase(Sheets(lCount2).Range("B5")) < UCase(Sheets(lCount).Range("B5")) Then
            Sheets(lCount2).Move Before:=Sheets(lCount)
        End If
    Next lCount2
Next lCount

'Select 3rd worksheet as active
Sheets(3).Select
Range("A1").Select
End Sub

Sub activateSheets()
'Activate Sheets
Dim i As Long
ActiveSheet.Select
For i = 2 To ThisWorkbook.Sheets.Count
    If Sheets(i).Name <> "Combine Sheet" And Sheets(i).Name <> "Standards" And Sheets(i).Name <> "Samples" Then Sheets(i).Select
    Replace:=False
Next i
End Sub

Sub Chart8786()
Dim oChtObj As ChartObject
Set oChtObj = ActiveSheet.ChartObjects.Add(Left:=0, Width:=465, Top:=355, Height:=105)
With oChtObj.Chart
    .ChartType = xlXYScatter
    .SetSourceData Source:=ActiveSheet.Range("j6:k56")
    .SeriesCollection(1).XValues = Range("j6:j50")
    .SeriesCollection(1).Values = Range("k6:k50")
    .SeriesCollection(1).Name = "ratio"
    'format
    .SeriesCollection(1).Border.ColorIndex = 1
    .SeriesCollection(1).Border.Weight = xlThin
    .SeriesCollection(1).Border.LineStyle = xlNone
    .SeriesCollection(1).MarkerBackgroundColorIndex = 5
    .SeriesCollection(1).MarkerForegroundColorIndex = 1
    .SeriesCollection(1).MarkerStyle = xlCircle
    .SeriesCollection(1).MarkerSize = 6
    'newseries
    .SeriesCollection.NewSeries
    .SeriesCollection(2).XValues = Range("")
    .SeriesCollection(2).Values = Range("j51:k52")
    .SeriesCollection(2).Name = "mean"
    'format
    .SeriesCollection(2).Border.ColorIndex = 1
    .SeriesCollection(2).Border.Weight = xlMedium
    .SeriesCollection(2).Border.LineStyle = xlDash
    .SeriesCollection(2).MarkerBackgroundColorIndex = 5
    .SeriesCollection(2).MarkerForegroundColorIndex = 1
    .SeriesCollection(2).MarkerStyle = xlNone
    .SeriesCollection(2).MarkerSize = 6
    'newseries
    .SeriesCollection.NewSeries
    .SeriesCollection(3).XValues = Range("j53:j54")
Sub ChartRb85V()
    Dim oChObj As ChartObject
    Set oChObj = ActiveSheet.ChartObjects.Add(Left:=0, Width:=465, Top:=568, Height:=80)
    With oChObj.Chart
        .ChartType = xlXYScatter
        .SetSourceData Source:=ActiveSheet.Range("j6:j50, o6:o50")
        .SeriesCollection(1).XValues = Range("j6:j50")
        .SeriesCollection(1).Values = Range("o6:o50")
        .SeriesCollection(1).Name = "85Rb(V)"
        .SeriesCollection(1).Border.ColorIndex = 4
        .SeriesCollection(1).Border.Weight = xlThick
        .SeriesCollection(1).Border.LineStyle = xlSolid
        .SeriesCollection(1).MarkerBackgroundColorIndex = 5
        .SeriesCollection(1).MarkerForegroundColorIndex = 1
        .SeriesCollection(1).MarkerStyle = xlNone
        .SeriesCollection(1).MarkerSize = 6
        .HasLegend = True
        .HasTitle = True
        .Axes(xlValue).TickLabels.NumberFormat = "0.00000"
        .Axes(xlValue).HasMajorGridlines = False
        .Axes(xlCategory).MinimumScale = 0
        .Axes(xlCategory).MaximumScale = 45
    End With
End Sub

Sub ChartKr86V()
    Dim oChObj As ChartObject
    Set oChObj = ActiveSheet.ChartObjects.Add(Left:=0, Width:=465, Top:=649, Height:=62)
    With oChObj.Chart
        .ChartType = xlXYScatter
        .SetSourceData Source:=ActiveSheet.Range("j6:j50, o6:o50")
        .SeriesCollection(1).XValues = Range("j6:j50")
        .SeriesCollection(1).Values = Range("o6:o50")
        .SeriesCollection(1).Name = "86 Kr(V)"
        .SeriesCollection(1).Border.ColorIndex = 44
        .SeriesCollection(1).Border.Weight = xlThick
        .SeriesCollection(1).Border.LineStyle = xlSolid
        .SeriesCollection(1).MarkerBackgroundColorIndex = 5
        .SeriesCollection(1).MarkerForegroundColorIndex = 1
        .SeriesCollection(1).MarkerStyle = xlNone
        .SeriesCollection(1).MarkerSize = 6
        .HasLegend = True
        .HasTitle = True
        .Axes(xlValue).TickLabels.NumberFormat = "0.00000"
        .Axes(xlValue).HasMajorGridlines = False
        .Axes(xlCategory).MinimumScale = 0
    End With
End Sub
Set oRange = Nothing
Set oChObj = Nothing

End Sub

Sub ChartBckgrnd()
    Dim oChObj As ChartObject
    Set oChObj = ActiveSheet.ChartObjects.Add(Left:=0, Width:=465, Top:=1200, Height:=105)
    With oChObj.Chart
        .ChartType = xlXYScatter
        .SetSourceData Source:=ActiveSheet.Range("q6:q90, r6:r90")
        .SeriesCollection(1).XValues = Range("q6:q90")
        .SeriesCollection(1).Values = Range("r6:r90")
        .SeriesCollection(1).Name = "88Sr(V)"
        .SeriesCollection(1).Border.ColorIndex = 29
        .SeriesCollection(1).Border.Weight = xlThick
        .SeriesCollection(1).Border.LineStyle = xlSolid
        .SeriesCollection(1).MarkerBackgroundColorIndex = 5
        .SeriesCollection(1).MarkerForegroundColorIndex = 1
        .SeriesCollection(1).MarkerStyle = xlNone
        .SeriesCollection(1).MarkerSize = 6

        .HasLegend = True
        .HasTitle = True
        .HasTitle = False
        .Axes(xlValue).TickLabels.NumberFormat = "0.000"
        .Axes(xlValue).HasMajorGridlines = False
        .Axes(xlCategory).MinimumScale = 0
    End With
    Set oRange = Nothing
Set oChObj = Nothing
End Sub