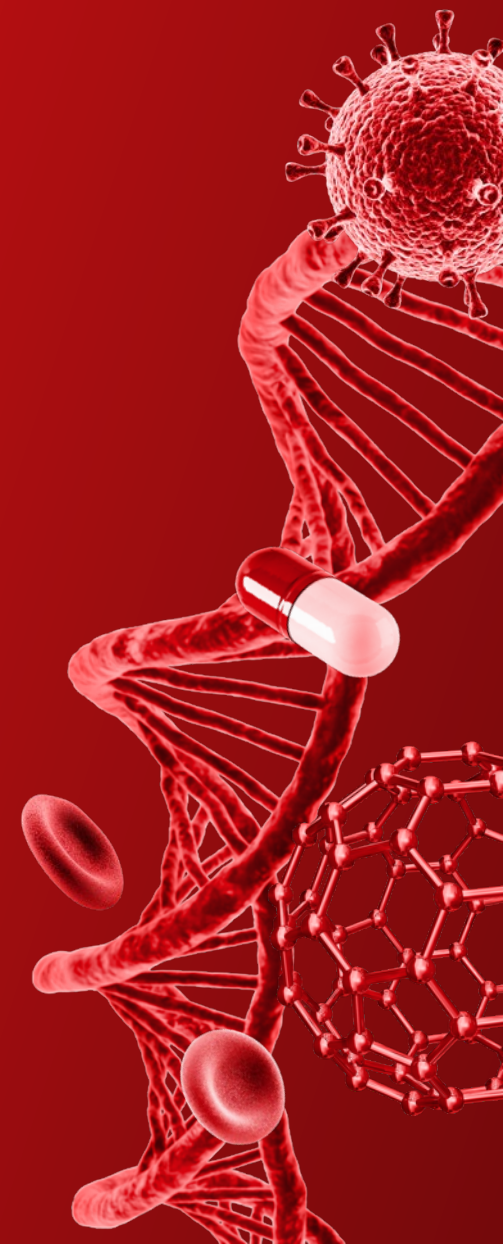


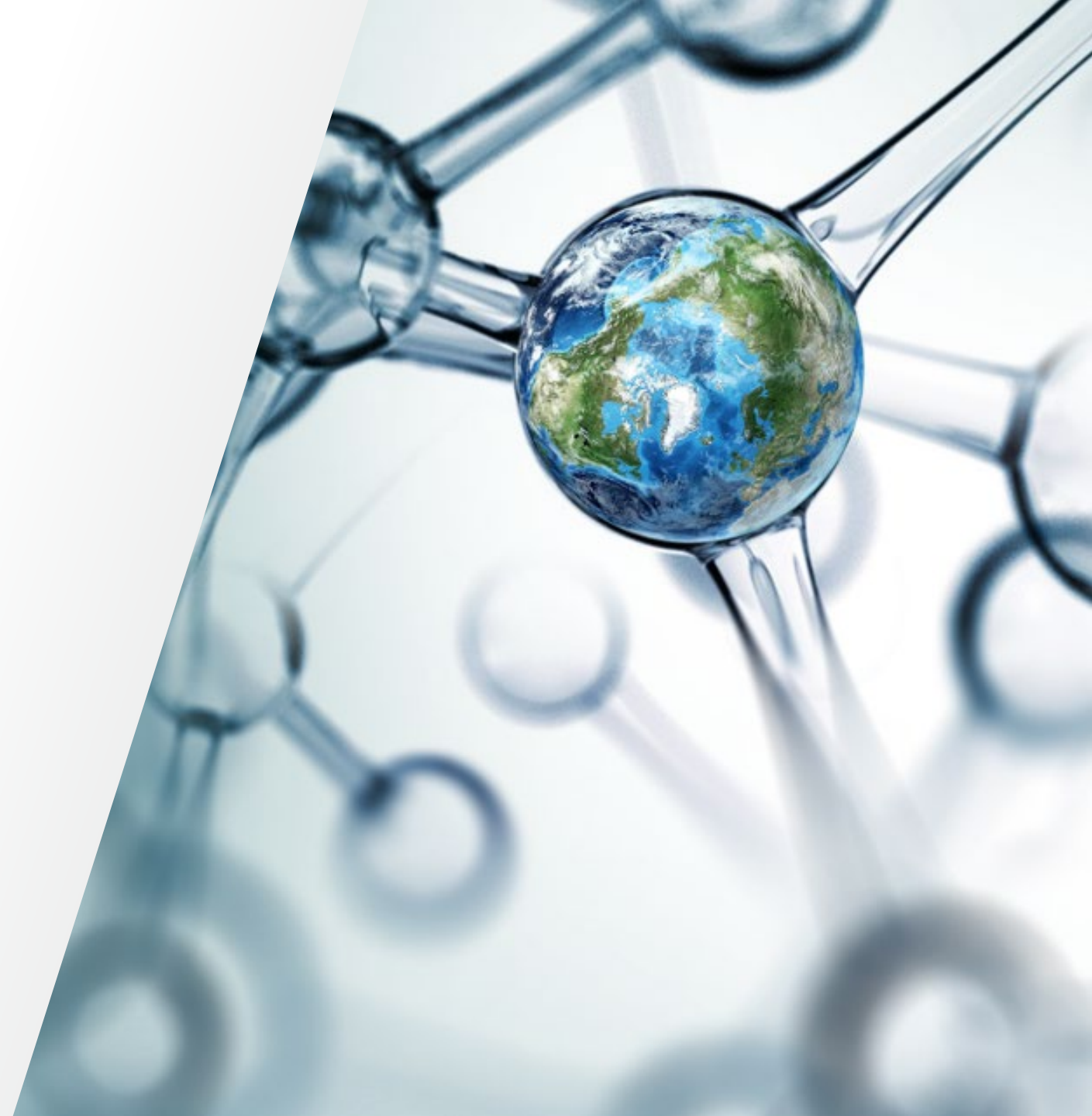
Welcome



Thermo Scientific™ Neoma™ MS/MS: The future of MC-ICP-MS

Darren Tollstrup, Grant Craig, Claudia Bouman

 The world leader in serving science



Triple Quadrupole ICP-MS/MS

New applications in related sector

- 2012 saw the launch of the first triple quadrupole ICPMS
- Thermo Scientific™ iCAP TQ™ ICP-MS/MS.
- Development of new applications in geoscience and bioscience
- Ability to remove isobaric and molecular interferences
- Some of these applications, are useful for quantitative analysis, but many (such as *in-situ* Rb/Sr dating, Ti, and Cr) would greatly benefit from the increased precision afforded by MC-ICP-MS.
- This sparked interest in the idea of a 'Triple Quad' MC-ICP-MS.



Plan A – Thermo Scientific *Proteus* MC-ICP-MS/MS

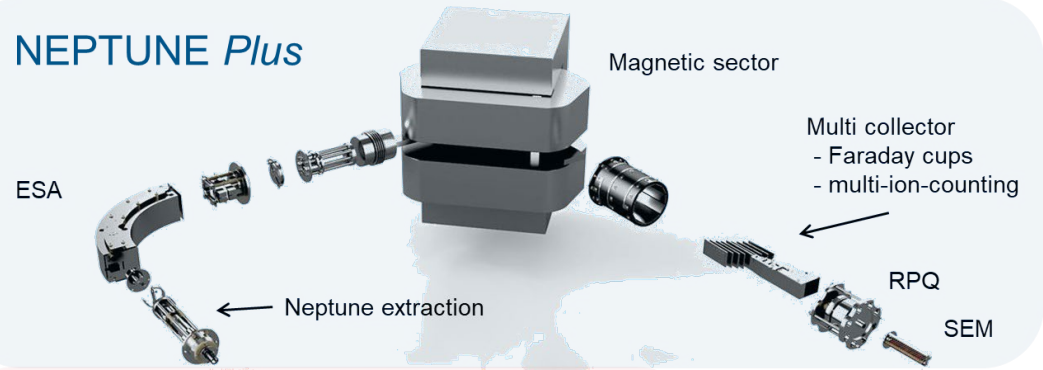
Everything we need can be found in our existing technologies



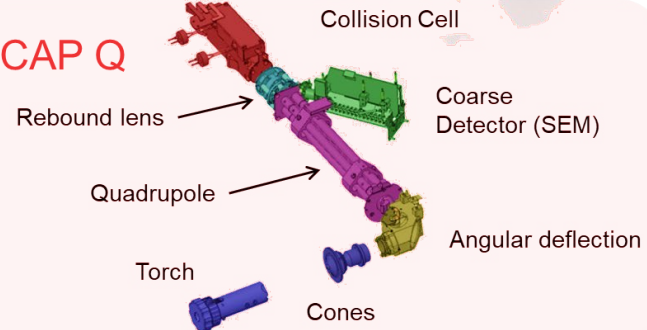
- Initial Prototype in collaboration with Tim Elliott at the University of Bristol.

Plan A – Thermo Scientific *Proteus* MC-ICP-MS/MS

NEPTUNE *Plus*



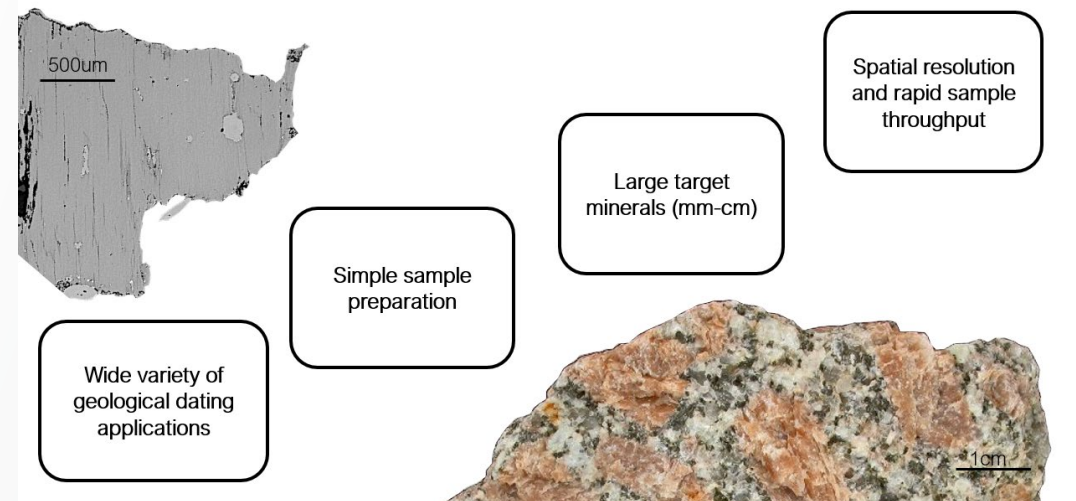
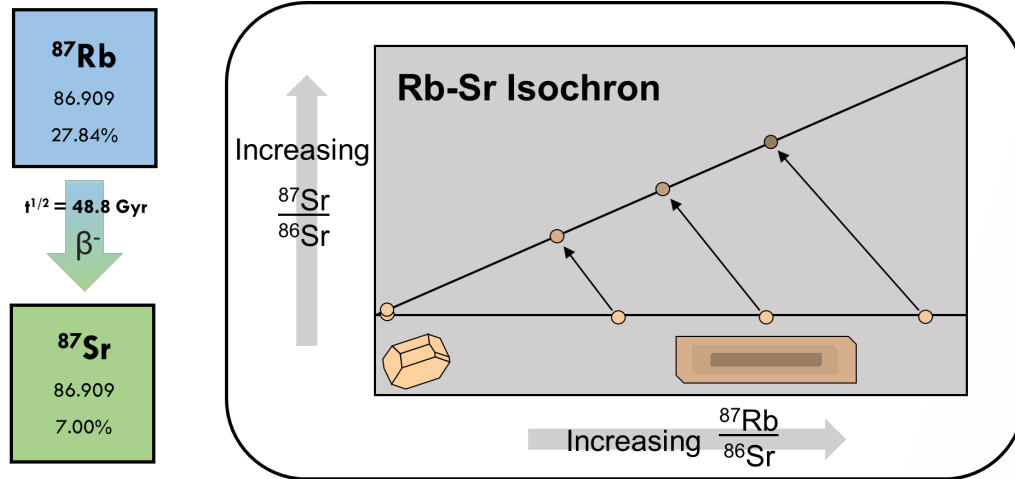
iCAP Q



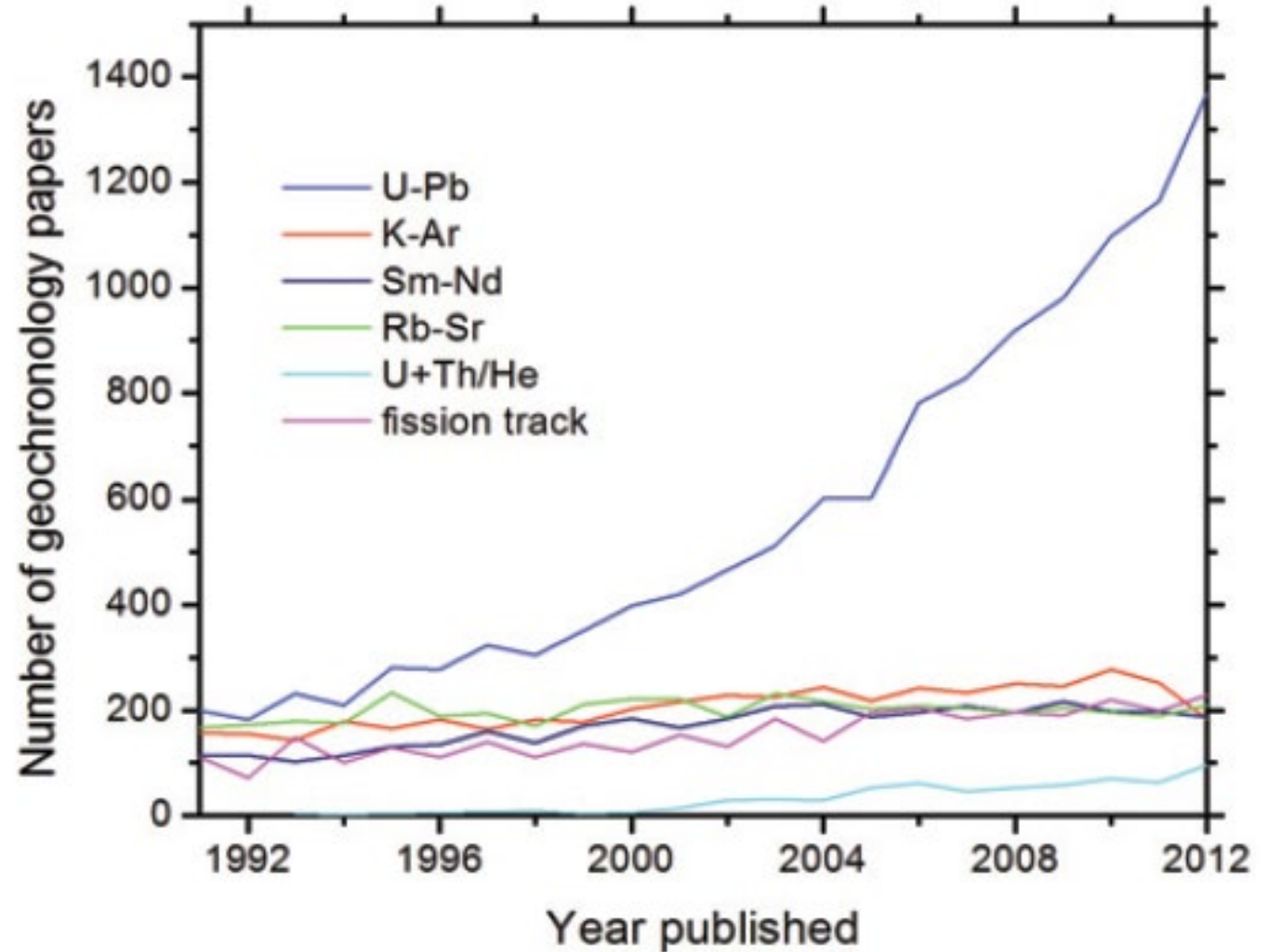
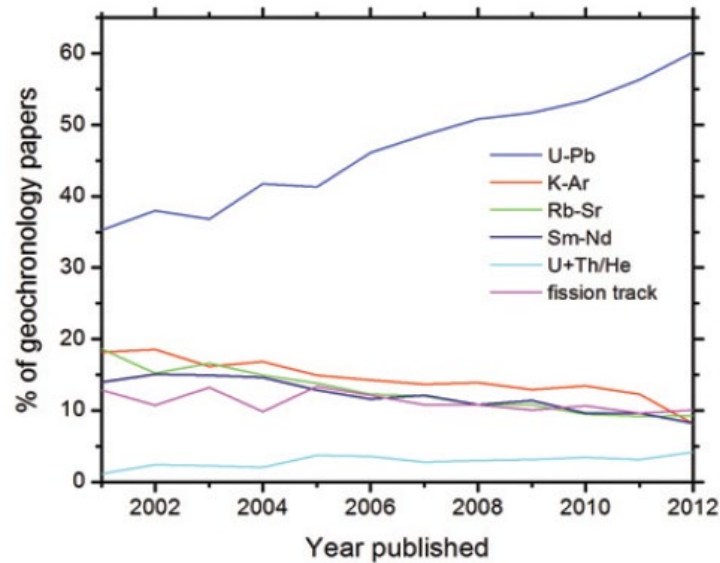
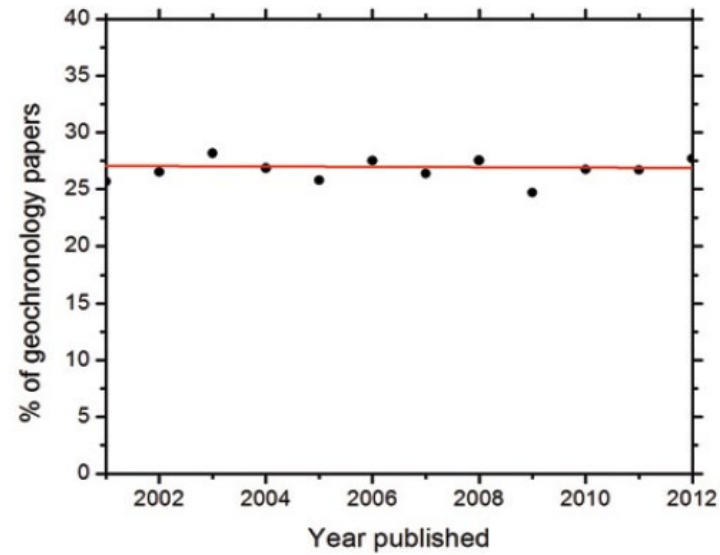
- A prototype tribrid instrument.
- Q1 retained before the collision/reaction cell, this pre-cell mass filter can control which masses enter the cell.

The Power of Proteus

- Unique capability: *in-situ* Rb-Sr dating by LA-MC-ICP-MS/MS
- SF_6 used as a reaction gas to form SrF , Rb does not react.
- Narrow mass window used to remove a variety of interferences:
 - $^{40}\text{Ar}^+$, $^{40}\text{Ar}^{16}\text{O}^+$, $^{40}\text{Ar}^{40}\text{Ar}^+$, $^{103}\text{Rh}^+$, $^{104}\text{Pd}^+$, $^{105}\text{Pd}^+$, $^{106}\text{Pd}^+$, $^{106}\text{Cd}^+$ and $^{107}\text{Ag}^+$

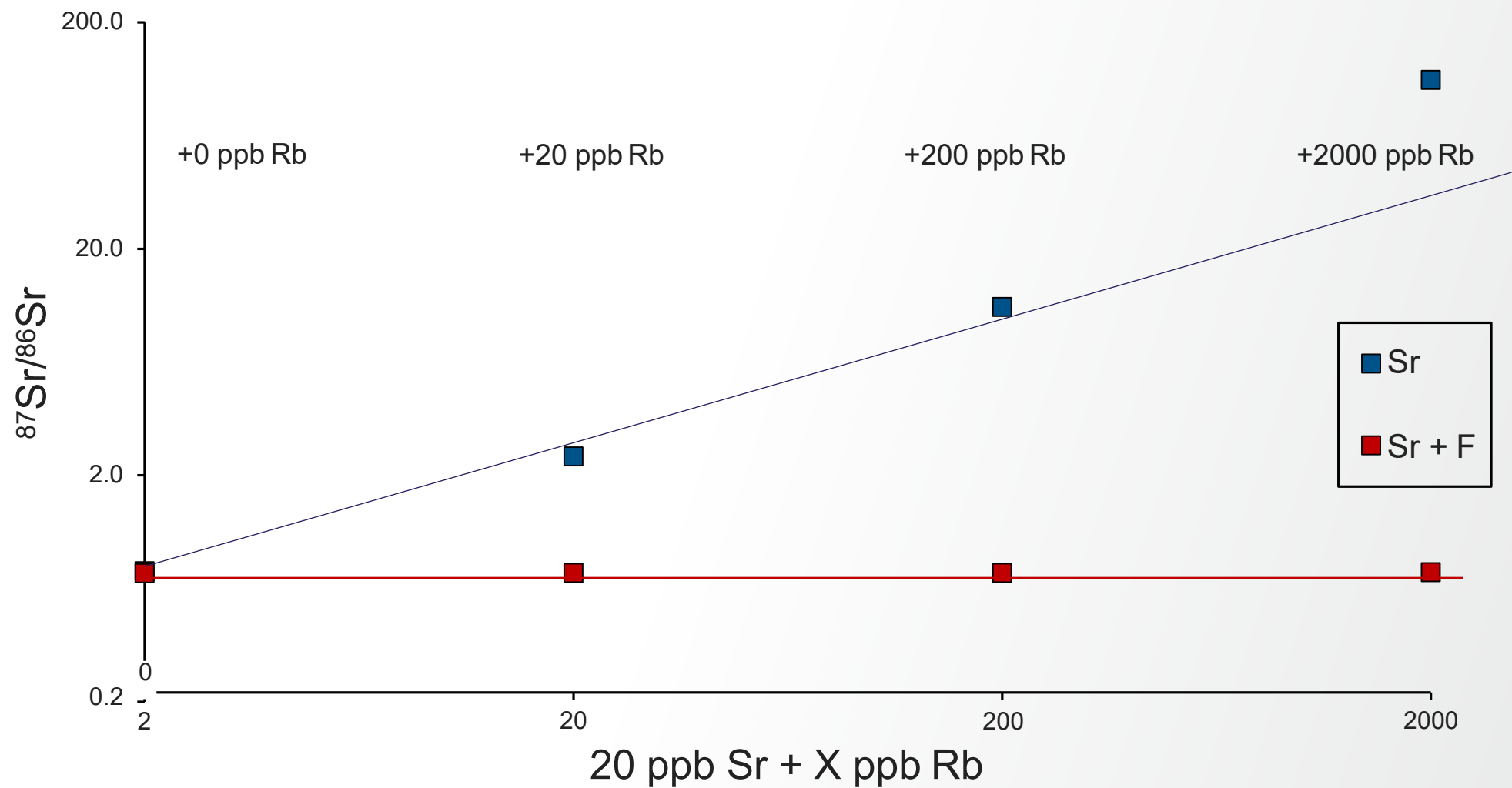


Neoma MS/MS: Geochronology

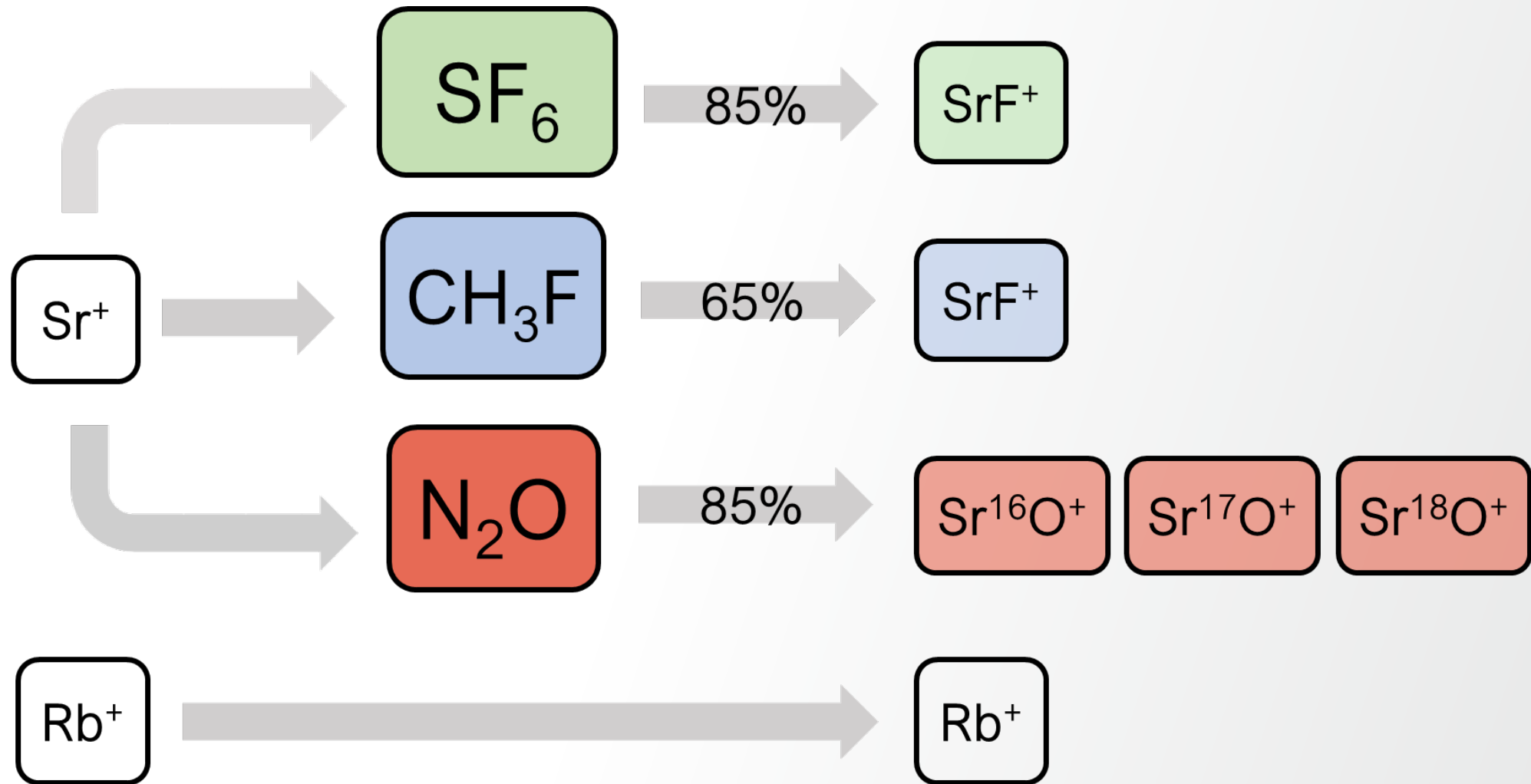


- Harrison, et al. 2015.

Neoma MS/MS: in-situ laser ablation Rb/Sr dating

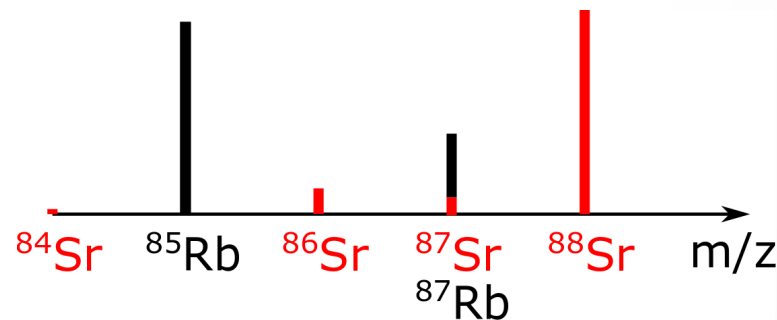


in-situ laser ablation Rb/Sr dating

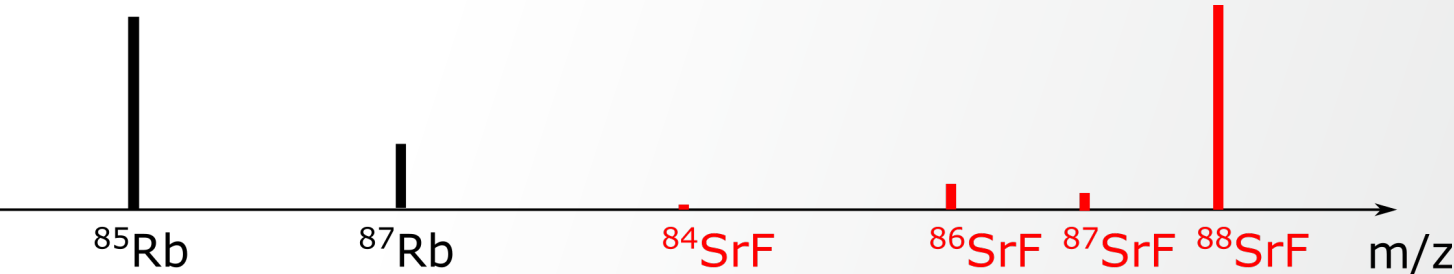


Separation of ⁸⁷Sr from ⁸⁷Rb

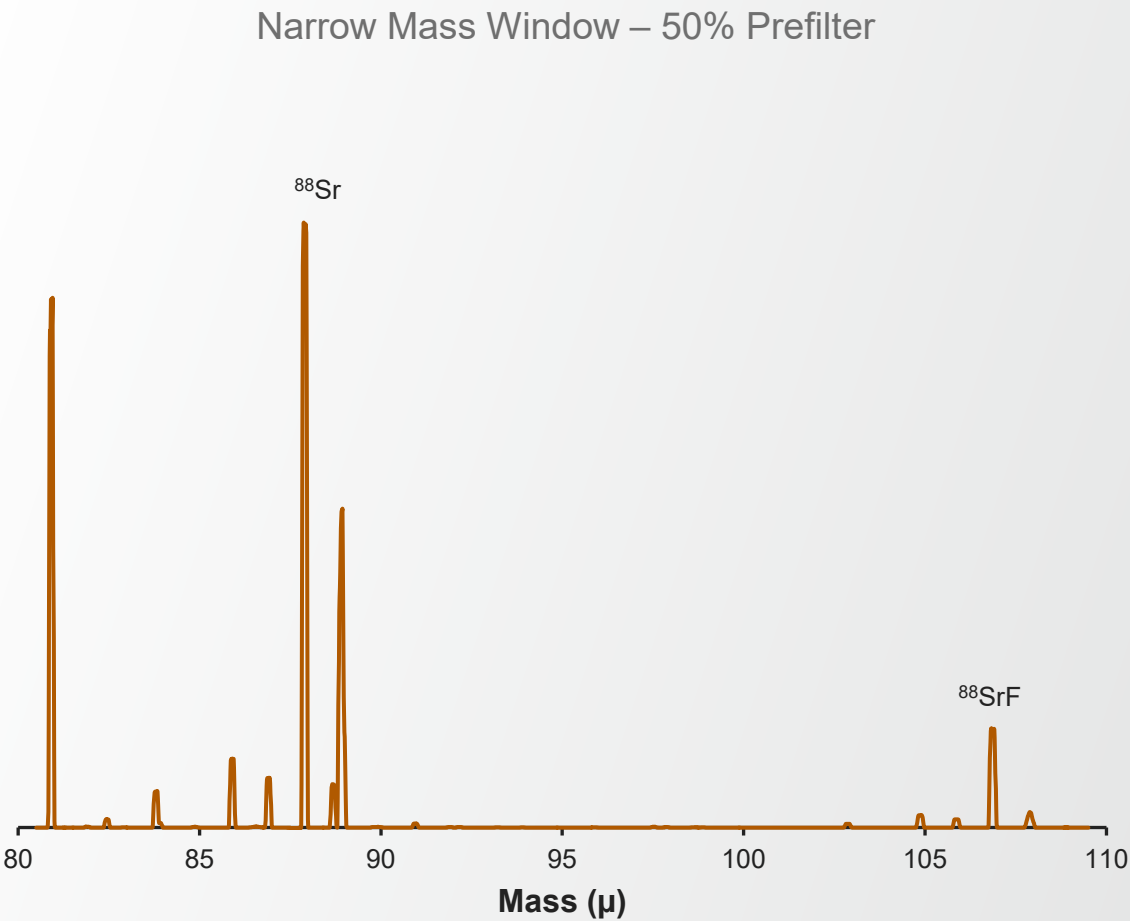
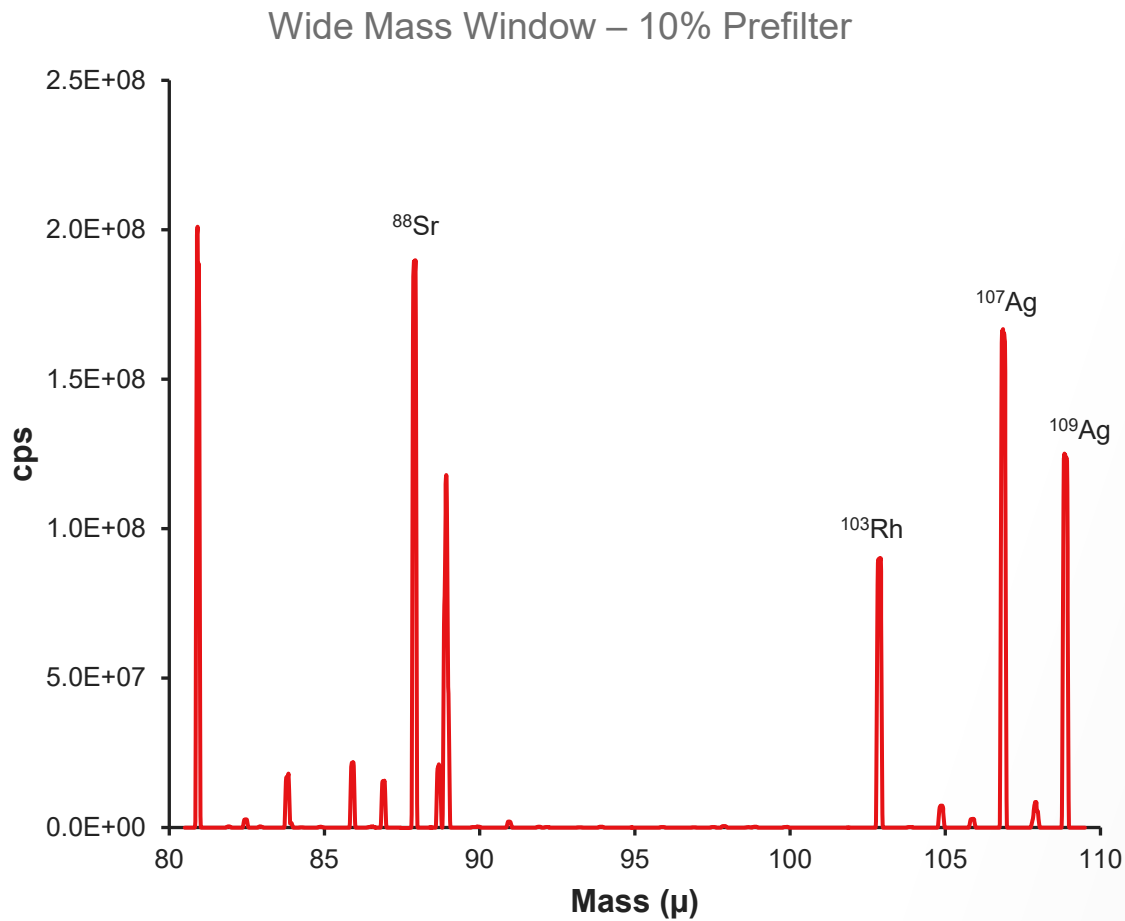
⁸⁷Sr reacts to form ⁸⁷SrF.



↓ CRC – reaction with SF₆

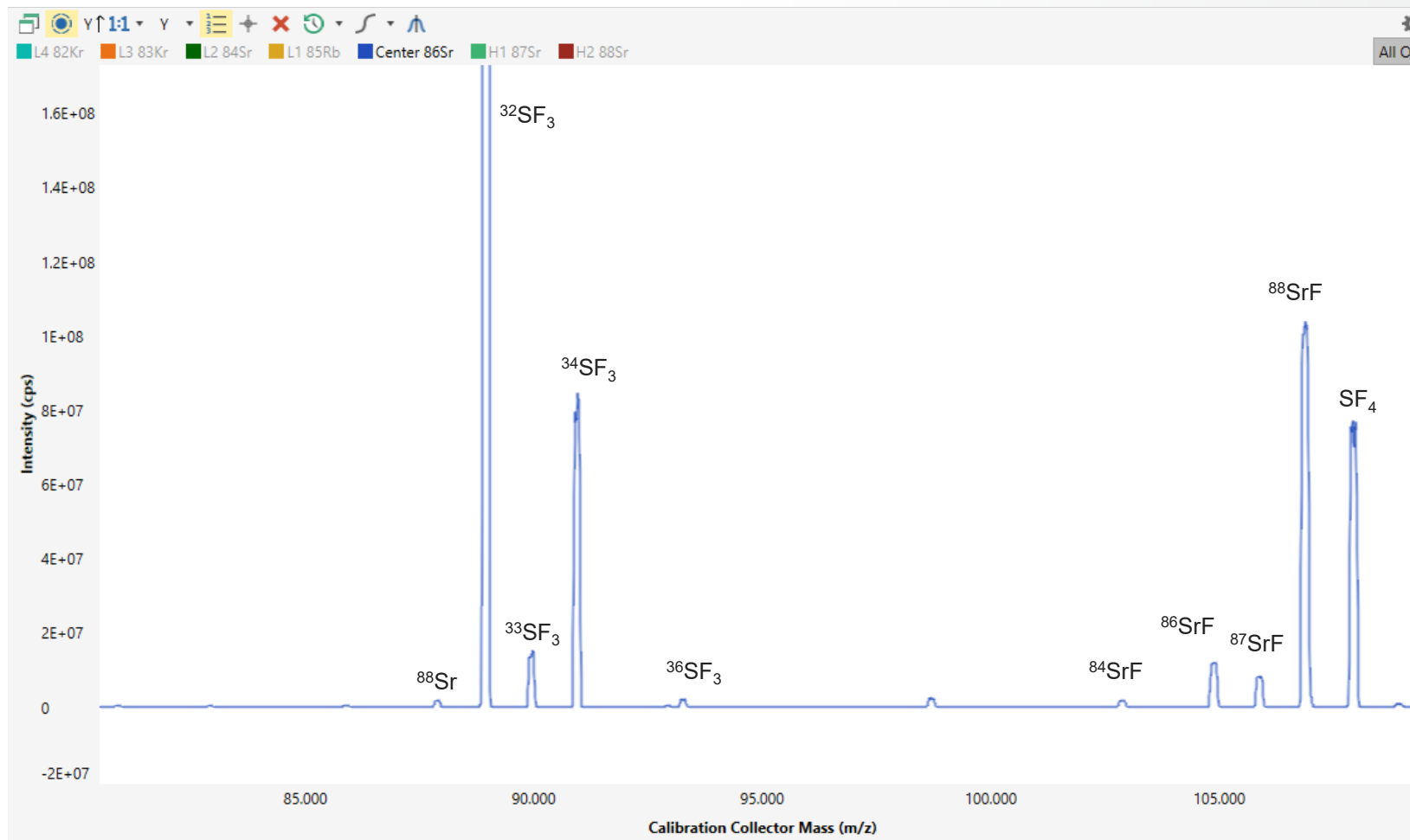


Cutting a mass window with trace SF₆ in collision/reaction cell: Solution contains Sr, Y, Rh and Ag.

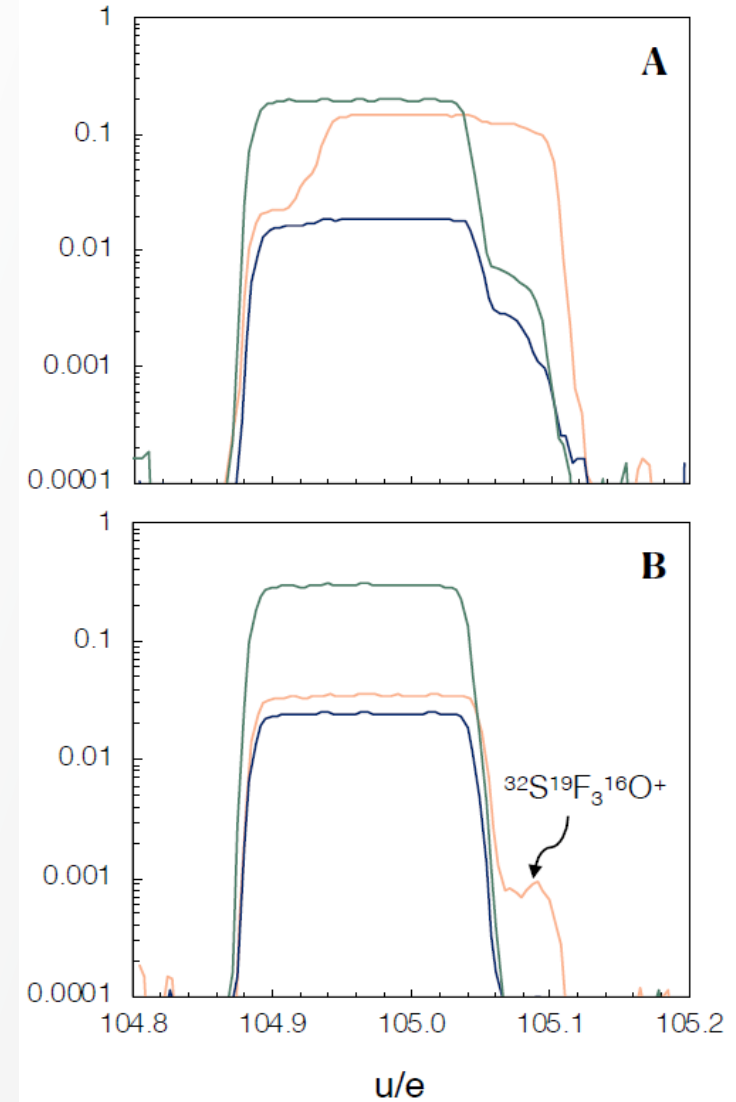
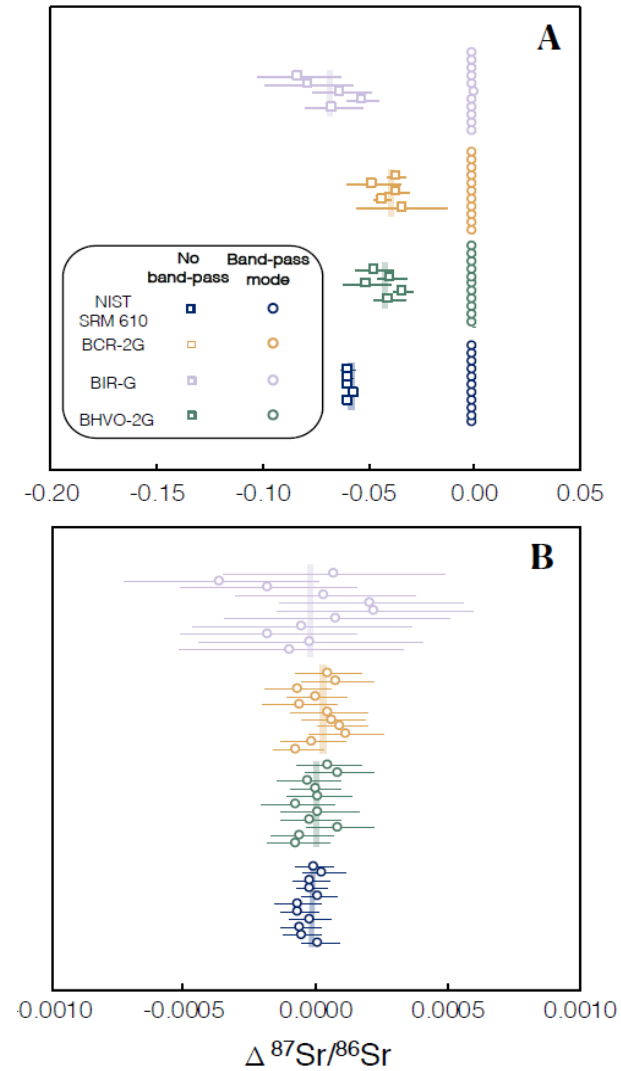
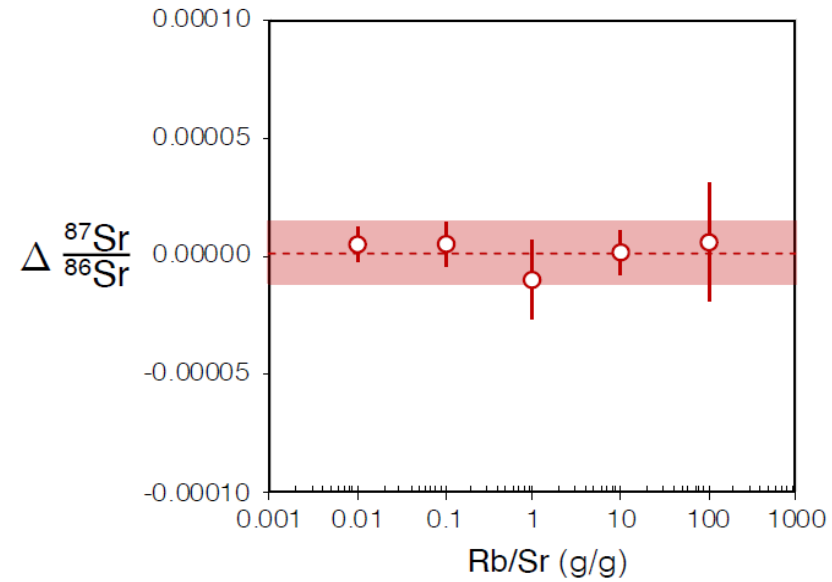


Adding more SF₆

Sr reacts to form SrF. >95% reaction efficiency.



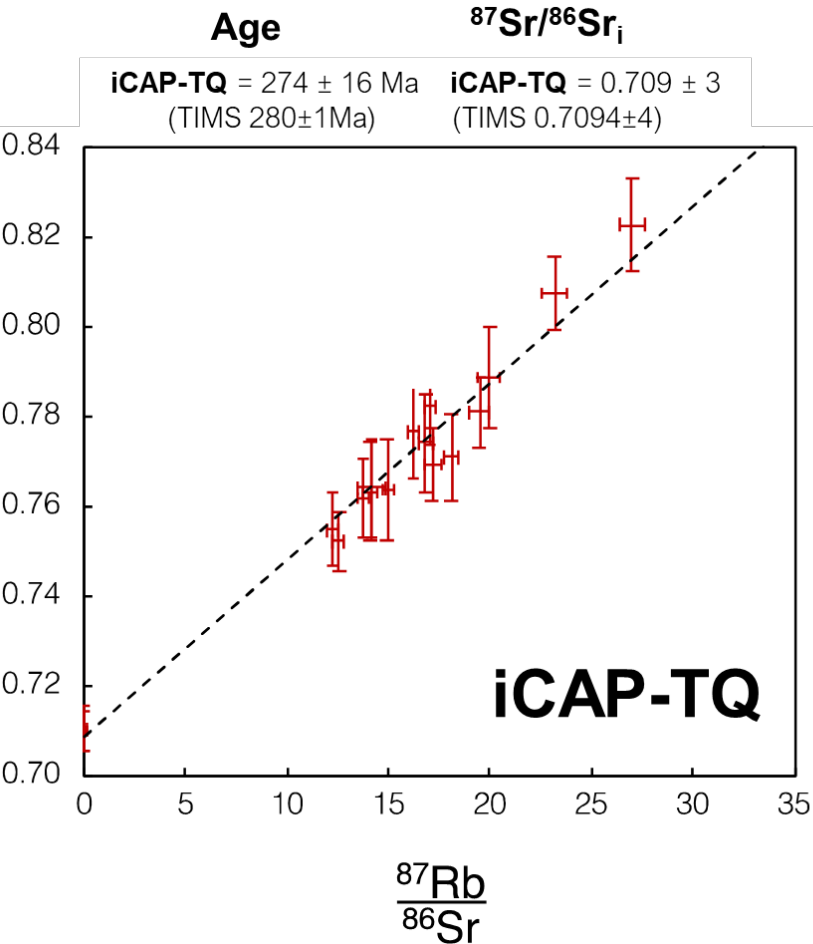
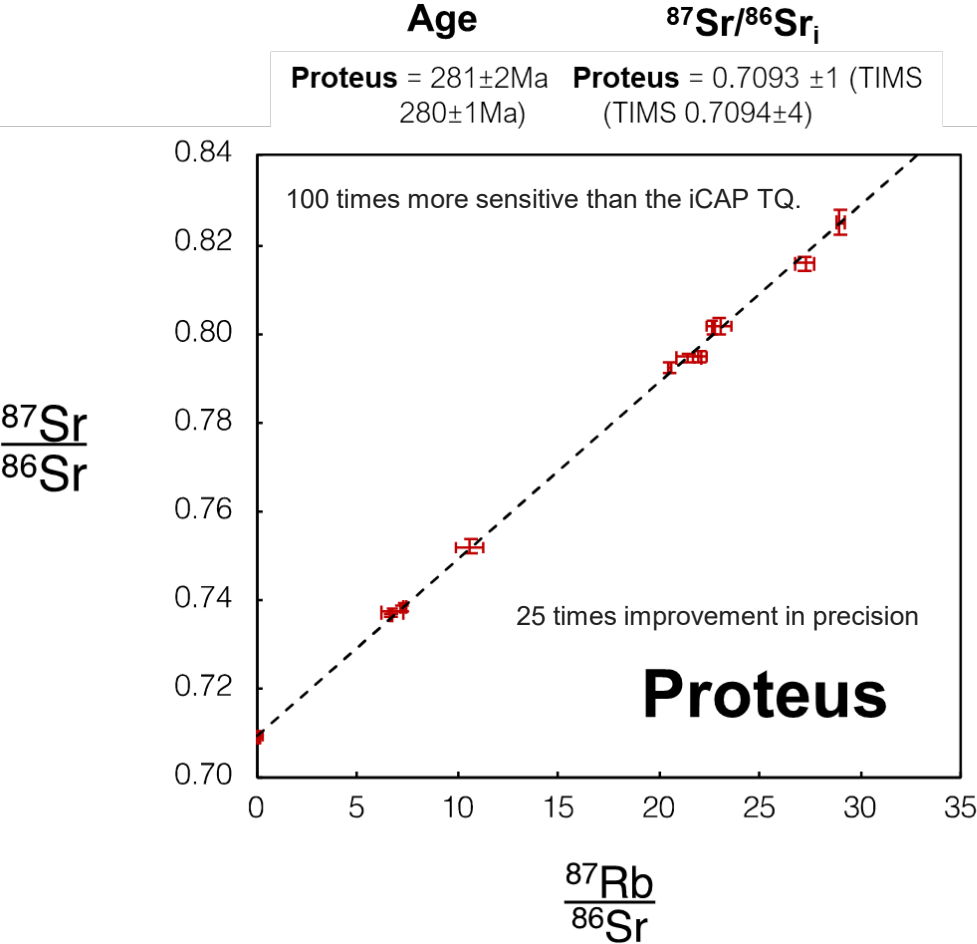
The Power of *Proteus*



1. Bevan, D.; Coath, C. D.; Lewis, J.; Schwieters, J.; Lloyd, N.; Craig, G.; Wehrs, H.; Elliott, T. In Situ Rb–Sr Dating by Collision Cell, Multicollection Inductively-Coupled Plasma Mass-Spectrometry with Pre-Cell Mass-Filter, (CC-MC-ICPMS/MS). *J. Anal. At. Spectrom.* **2021**, *36*, 917–931.

Proteus vs iCAP-TQ

Dartmoor Granite: Proteus v iCAP-TQ¹



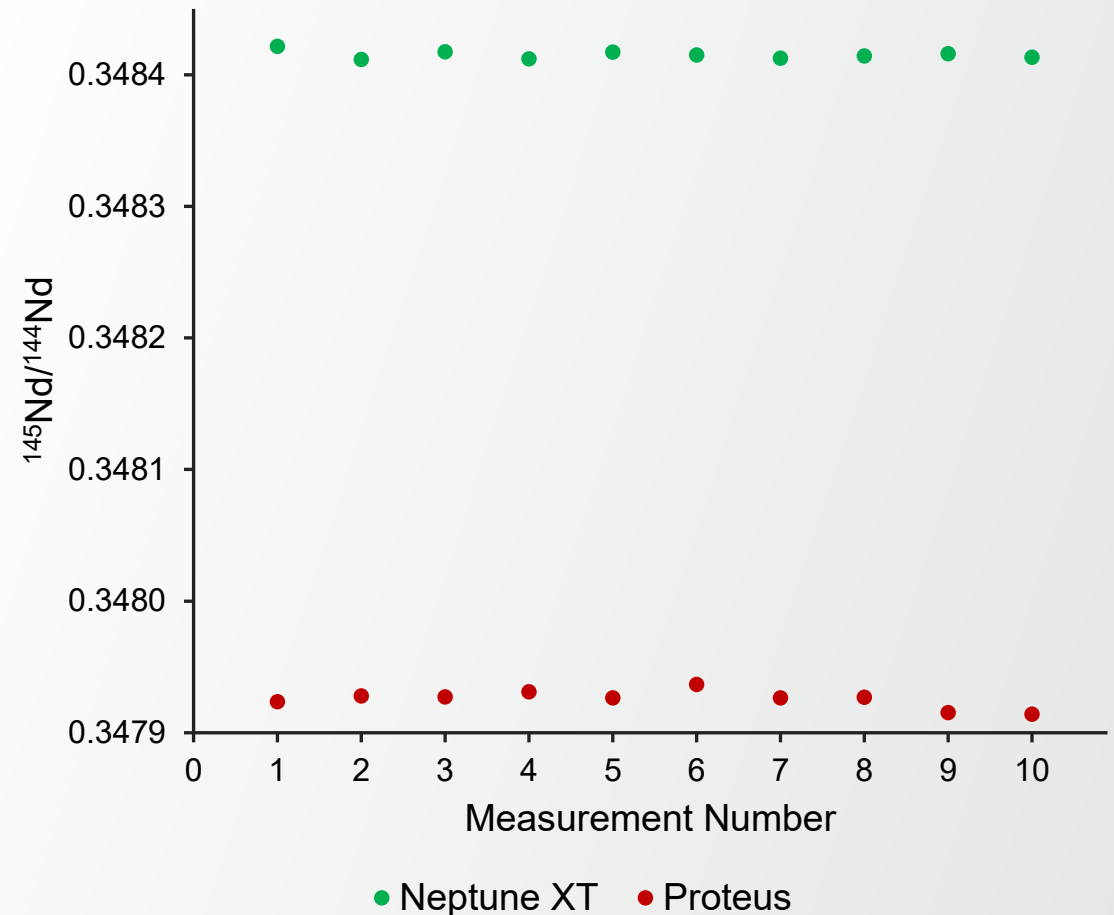
1. Bevan, D.; Coath, C. D.; Lewis, J.; Schwieters, J.; Lloyd, N.; Craig, G.; Wehrs, H.; Elliott, T. In Situ Rb–Sr Dating by Collision Cell, Multicollection Inductively-Coupled Plasma Mass-Spectrometry with Pre-Cell Mass-Filter, (CC-MC-ICPMS/MS). *J. Anal. At. Spectrom.* **2021**, 36, 917–931.

Why not *Proteus*?

Sensitivity and accuracy

Proteus was found to have two significant limitations which hindered further implementation of the design:

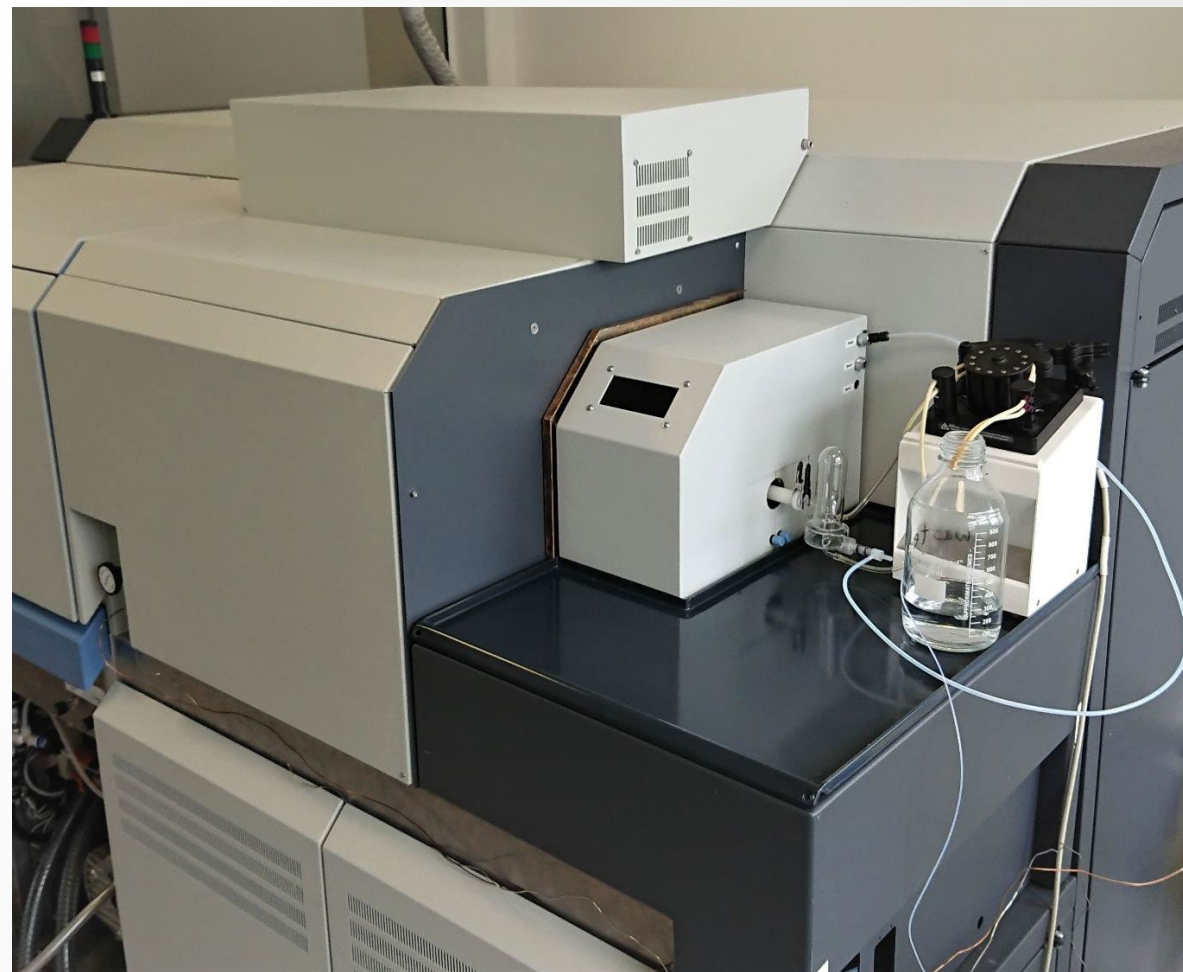
1. Limited sensitivity due to the low-energy extraction required for the operation of the Q1 pre-cell mass filter. Sensitivity was < 25% of what we expect from a typical MC-ICP-MS.
2. Inaccurate isotopic systems which rely on internally normalizing for the exponential mass bias of mass spectrometer. Q1 introduced non-exponential behavior, “nodding”.



Plan B – Thermo Scientific *Vienna* MC-ICP-MS/MS

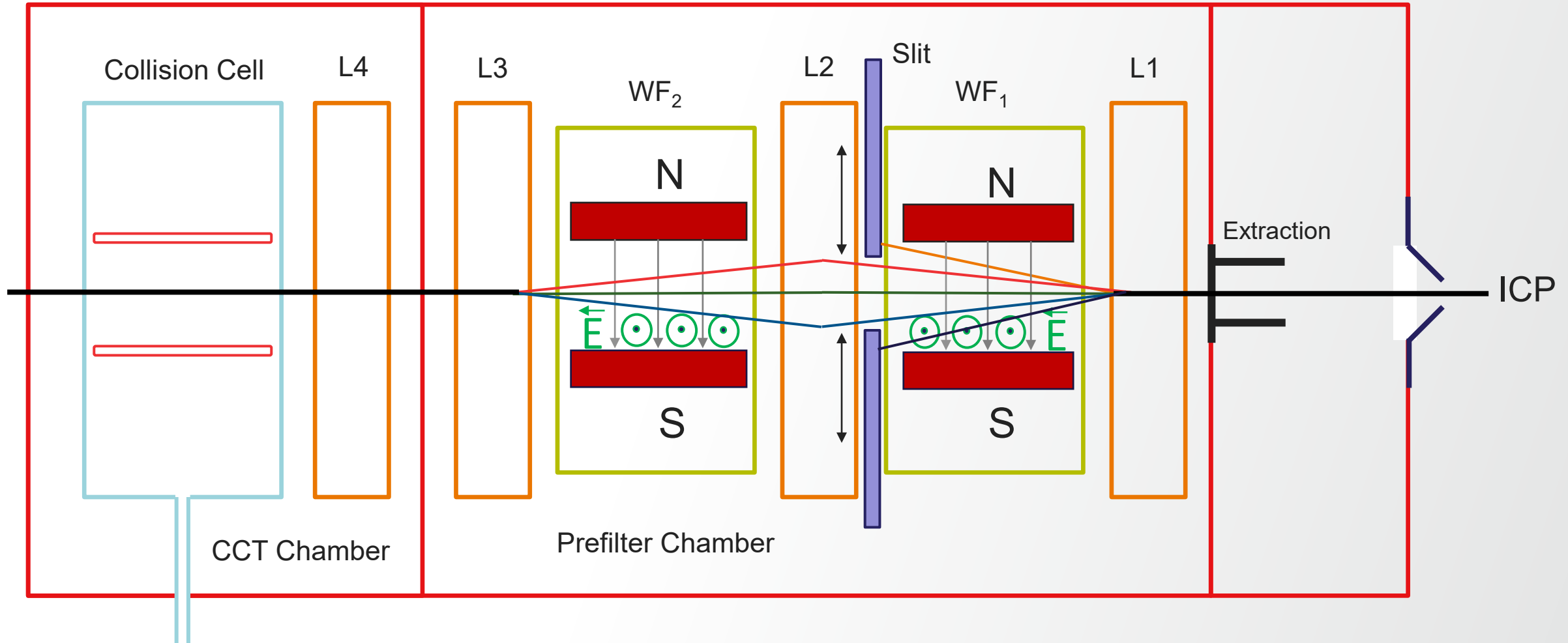
Moving away from quadrupoles – a unique pre-cell mass filter¹.

- To retain sensitivity and exponential mass bias characteristics, our ‘triple quad’ MC-ICP-MS/MS would need to abandon the Q1 pre-cell mass filter.
- A new pre-cell mass filter based on a dual Wien design was created.
- Prototype installed on a Neptune XT, resulting MC-ICP-MS/MS was named Vienna.
- Successfully retained sensitivity and exponential mass bias characteristics of the Neptune XT MC-ICP-MS.



Neoma MS/MS Option

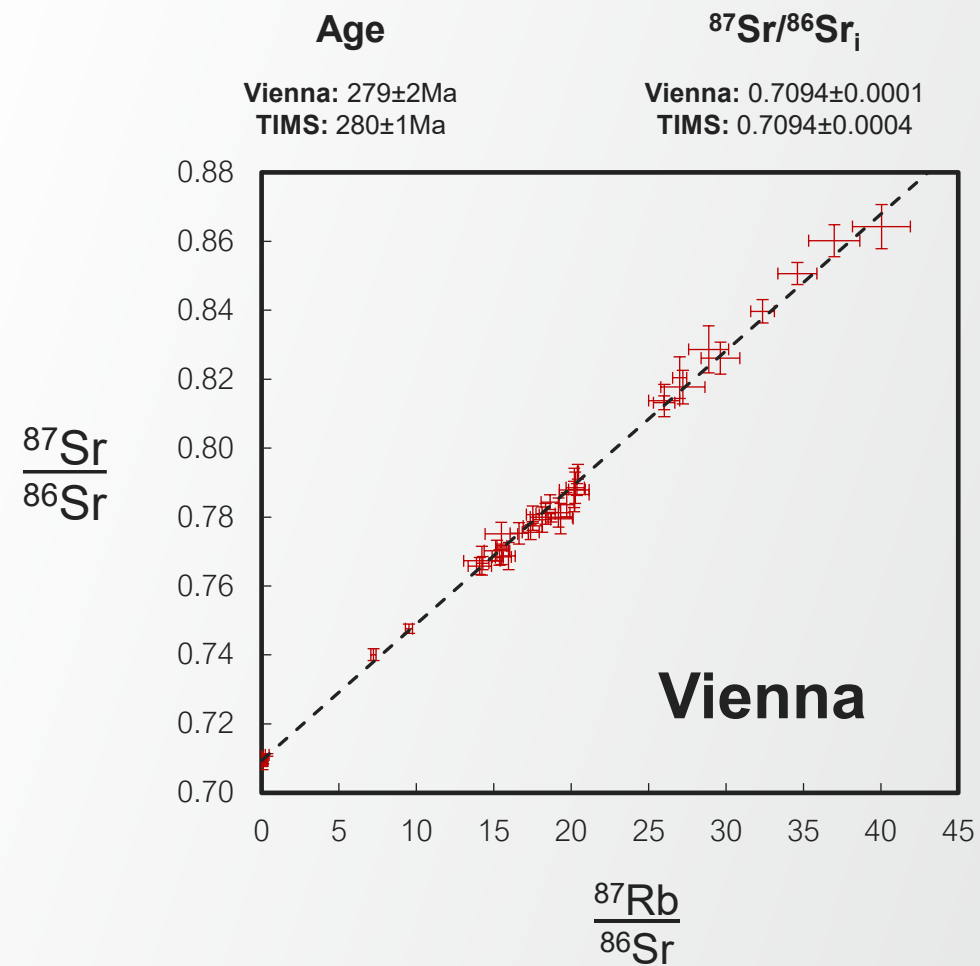
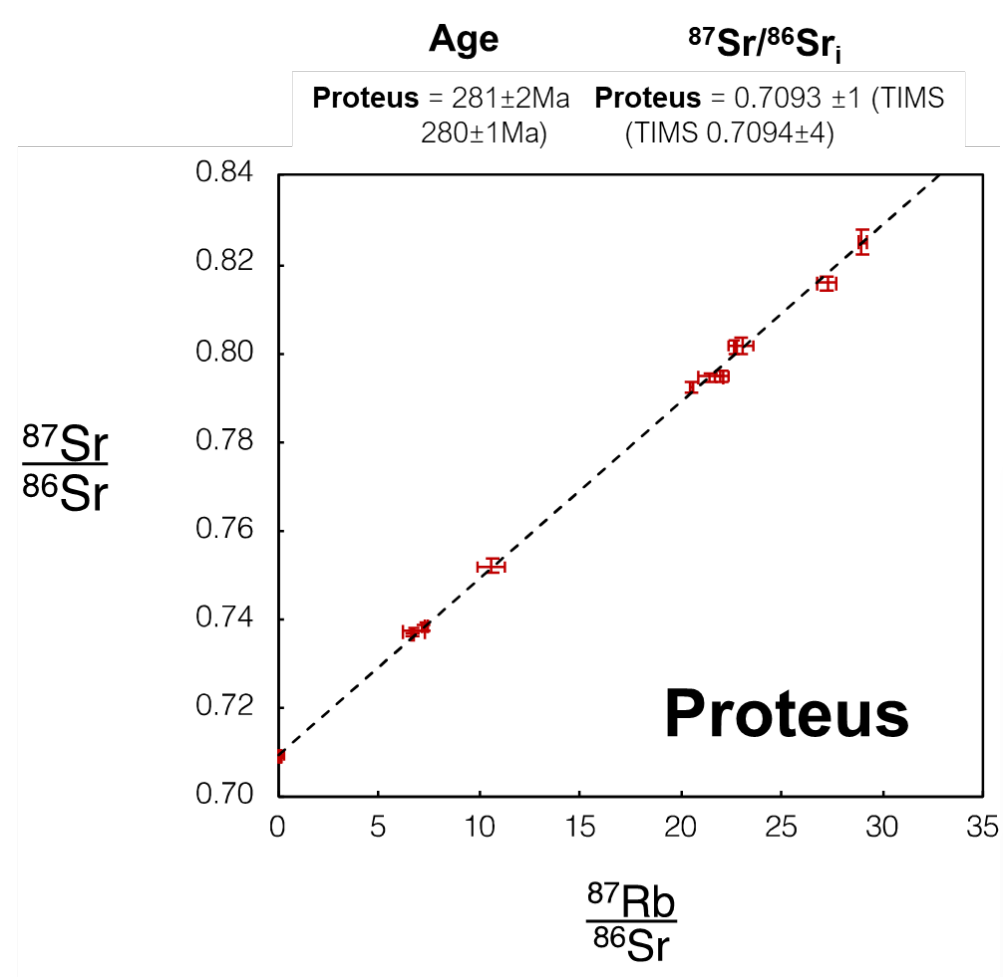
Based on prototype module developed on Thermo Scientific™ Vienna MC-ICP-MS/MS¹



1. Craig, G.; Wehrs, H.; Bevan, D. G.; Pfeifer, M.; Lewis, J.; Coath, C. D.; Elliott, T.; Huang, C.; Lloyd, N. S.; Schwieters, J. B. Project Vienna: A Novel Precell Mass Filter for Collision/Reaction Cell MC-ICPMS/MS. *Anal. Chem.* **2021**, 93 (30), 10519–10527.

Proteus v Vienna – *in-situ* Rb/Sr dating

Retained performance with new pre-cell mass filter.



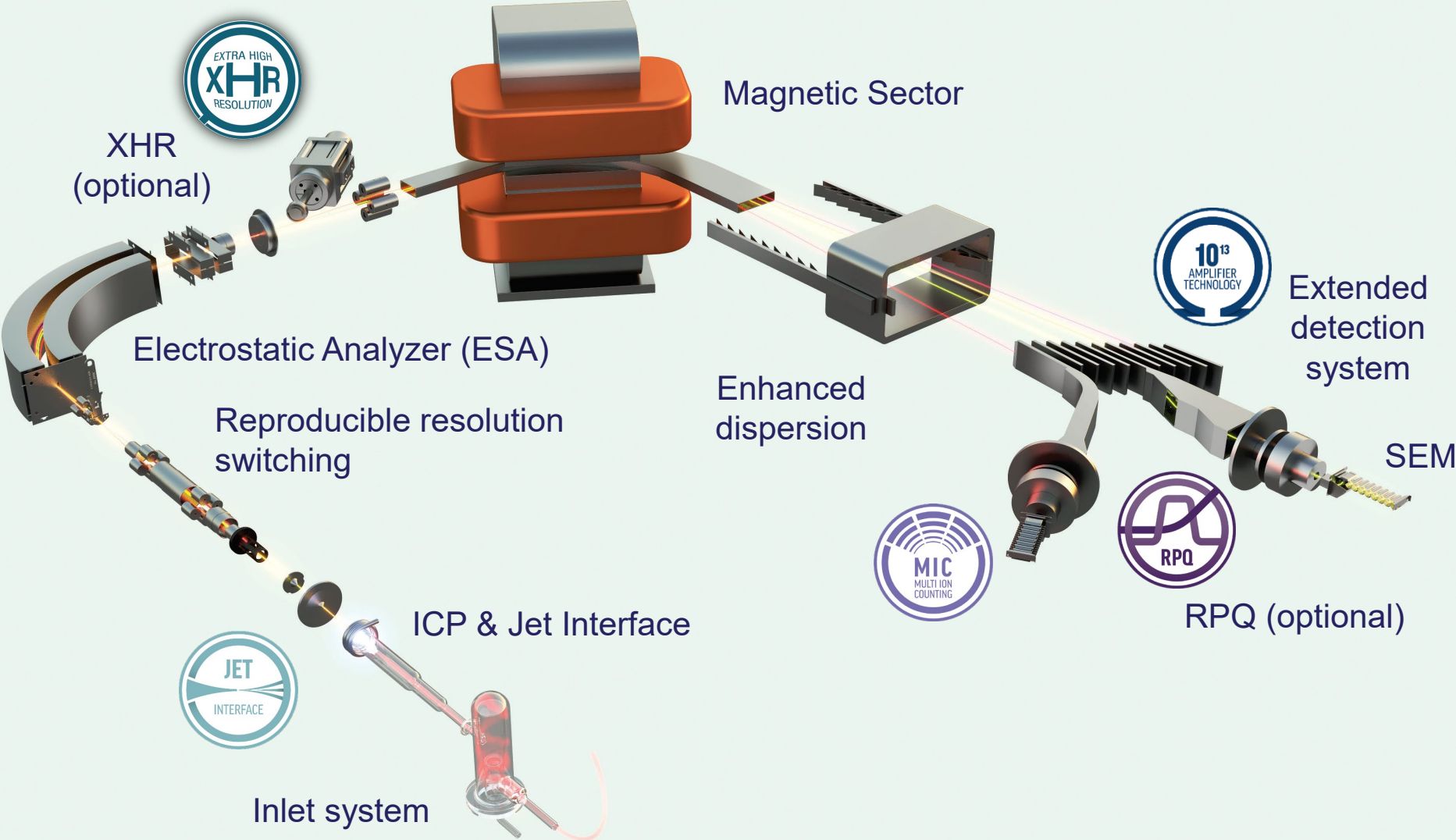
High-precision isotope ratio analysis, simplified.

ThermoFisher
SCIENTIFIC



Thermo Scientific™ Neoma™ MC-ICP-MS

MC-ICP-MS – Inside Neoma



Limit-breaking Detector Array



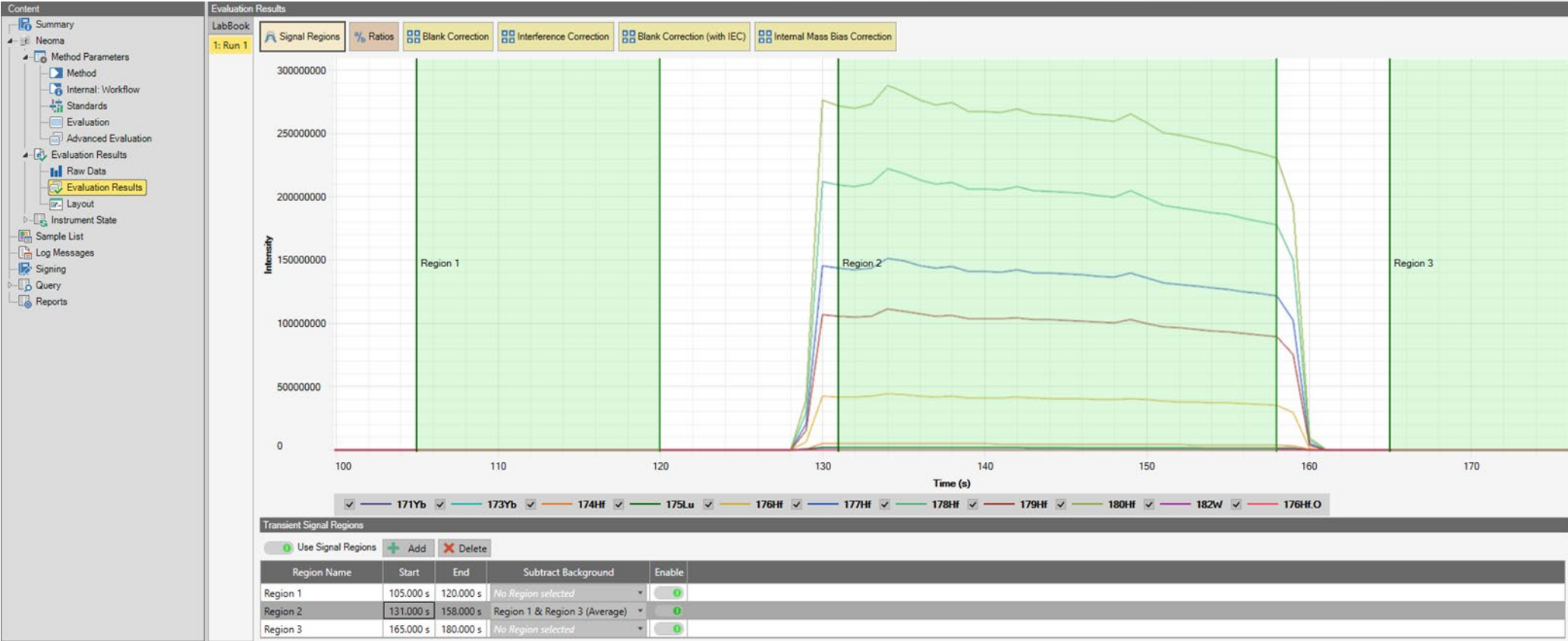
- Ultimate flexibility
 - 11 Faraday cups mobile detector array
 - >22% dispersion
 - No limitations
 - Automated Alignment.
 - 24 customizable amplifier slots
 - 10¹³ Ohm Amplifier Technology™ with extended dynamic range
 - Up to 100 V on 10¹¹ Ω and up to 1 V on 10¹³ Ω.
 - Multi Ion Counting options with dual RPQ for nuclear applications.
 - Dynamic measurements with extended dispersion lens optics.



	L5	L4	L3	L2	L1	C	H1	H2	H3	H4	H5
Mg/Si	²⁴ Mg		²⁵ Mg		²⁶ Mg	²⁷ Al	²⁸ Si		²⁹ Si		³⁰ Si
Si/S	²⁸ Si		²⁹ Si		³⁰ Si	³¹ P	³² S		³³ S		³⁴ S
Ca	⁴⁰ Ca	⁴¹ K	⁴² Ca	⁴³ Ca	⁴⁴ Ca	⁴⁵ Sc	⁴⁶ Ca	⁴⁷ Ti	⁴⁸ Ca		⁴⁹ Ti
Fe	⁵² Cr	⁵³ Cr	⁵⁴ Fe	⁵⁶ Fe	⁵⁷ Fe	⁵⁸ Fe	⁶⁰ Ni	⁶¹ Ni	⁶² Ni	⁶³ Cu	⁶⁵ Cu
Sr	⁸² Kr	⁸³ Kr	¹⁶⁷ Er ⁺⁺	⁸⁴ Sr	⁸⁵ Rb	¹⁷¹ Yb ⁺⁺	⁸⁶ Sr	¹⁷³ Yb ⁺⁺	⁸⁷ Sr	⁸⁸ Sr	¹⁷⁷ Hf ⁺⁺
Nd	¹⁴⁰ Ce	¹⁴² Nd	¹⁴³ Nd	¹⁴⁴ Nd	¹⁴⁵ Nd	¹⁴⁶ Nd	¹⁴⁷ Sm	¹⁴⁸ Nd	¹⁴⁹ Sm	¹⁵⁰ Nd	¹⁵¹ Eu
Hf	¹⁷¹ Yb	¹⁷³ Yb	¹⁷⁴ Hf	¹⁷⁵ Lu	¹⁷⁶ Hf	¹⁷⁷ Hf	¹⁷⁸ Hf	¹⁷⁹ Hf	¹⁸⁰ Hf	¹⁸¹ Ta	¹⁸² W
U/Pb	²⁰² Hg	²⁰⁴ Pb	²⁰⁶ Pb	²⁰⁷ Pb	²⁰⁸ Pb				²³² Th	²³⁵ U	²³⁸ U
Rb/Sr	⁸⁵ Rb	⁸⁶ Sr	⁸⁷ Rb	⁸⁸ Sr				⁸⁴ SrF	⁸⁶ SrF	⁸⁷ SrF	⁸⁸ SrF

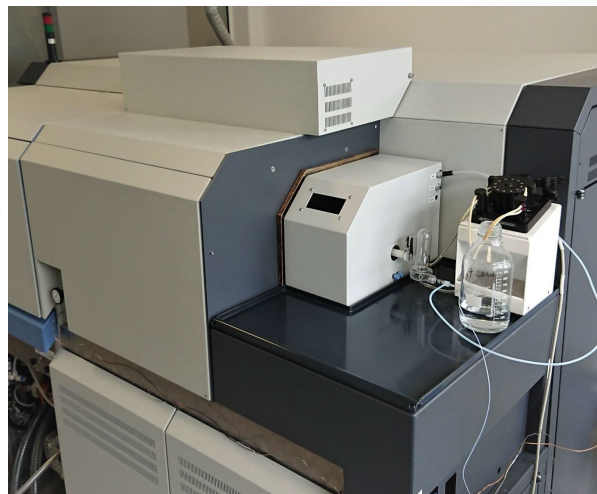
Laser Ablation – Data Processing

- Qtegra for Neoma can process transient signals – full data processing for *in-situ* Hf.



The Final Step – Thermo Scientific Neoma MS/MS

Transfer of technologies developed on Vienna to the new Neoma MC-ICP-MS platform



Triple Magnet: Adding the MS/MS Option to the Neoma MC-ICP-MS

MS/MS Option can be added to the Neoma MC-ICP-MS

- Before and After
- New MS/MS Module
- Field Upgradeable



- 4 Mass Flow Controllers (MFCs)
- Reactive and Collision Gases
- Fully integrated.



Neoma MC-ICP-MS at TFS Bremen

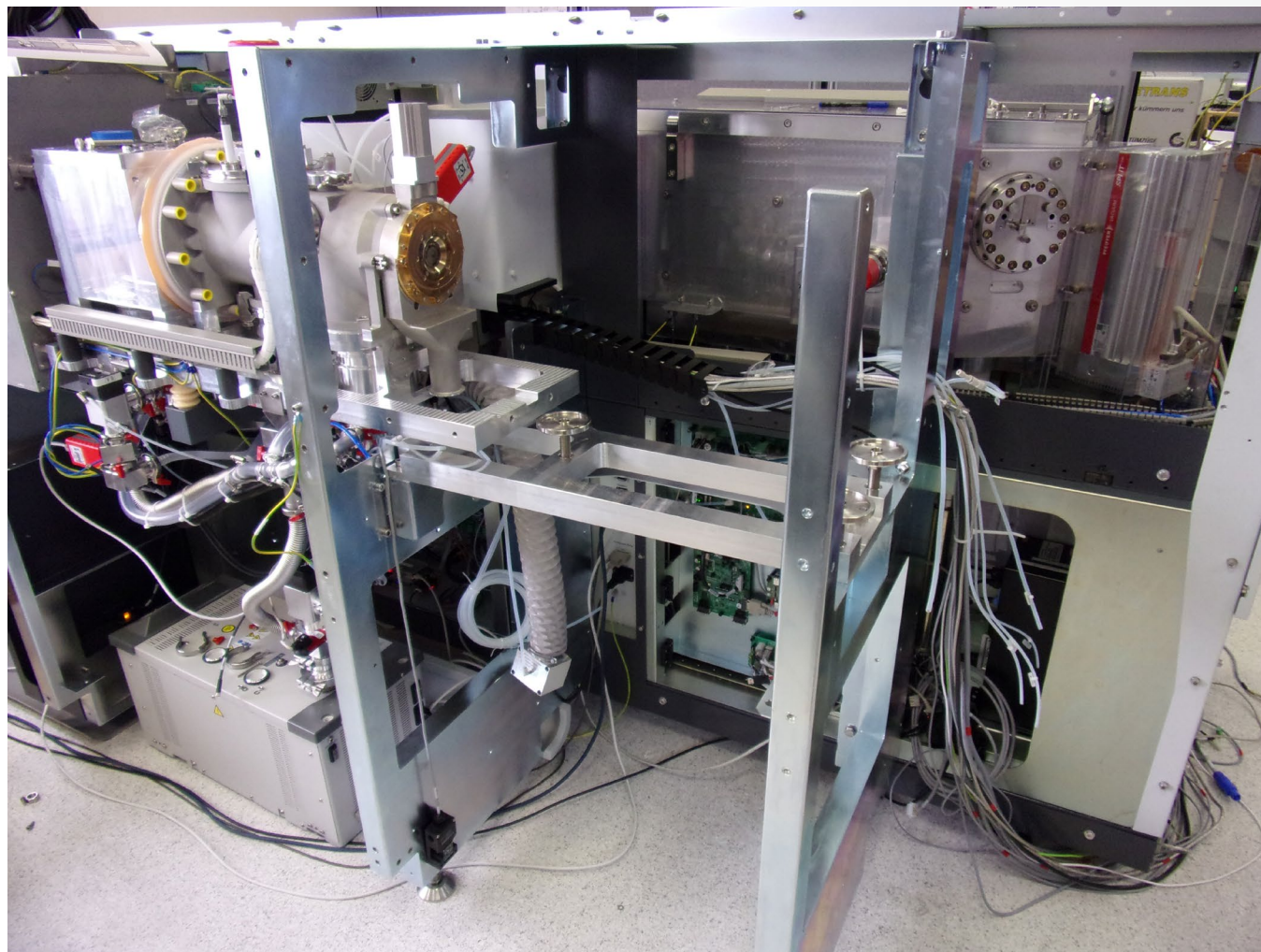


Neoma MC-ICP-MS with MS/MS Option at TFS Bremen

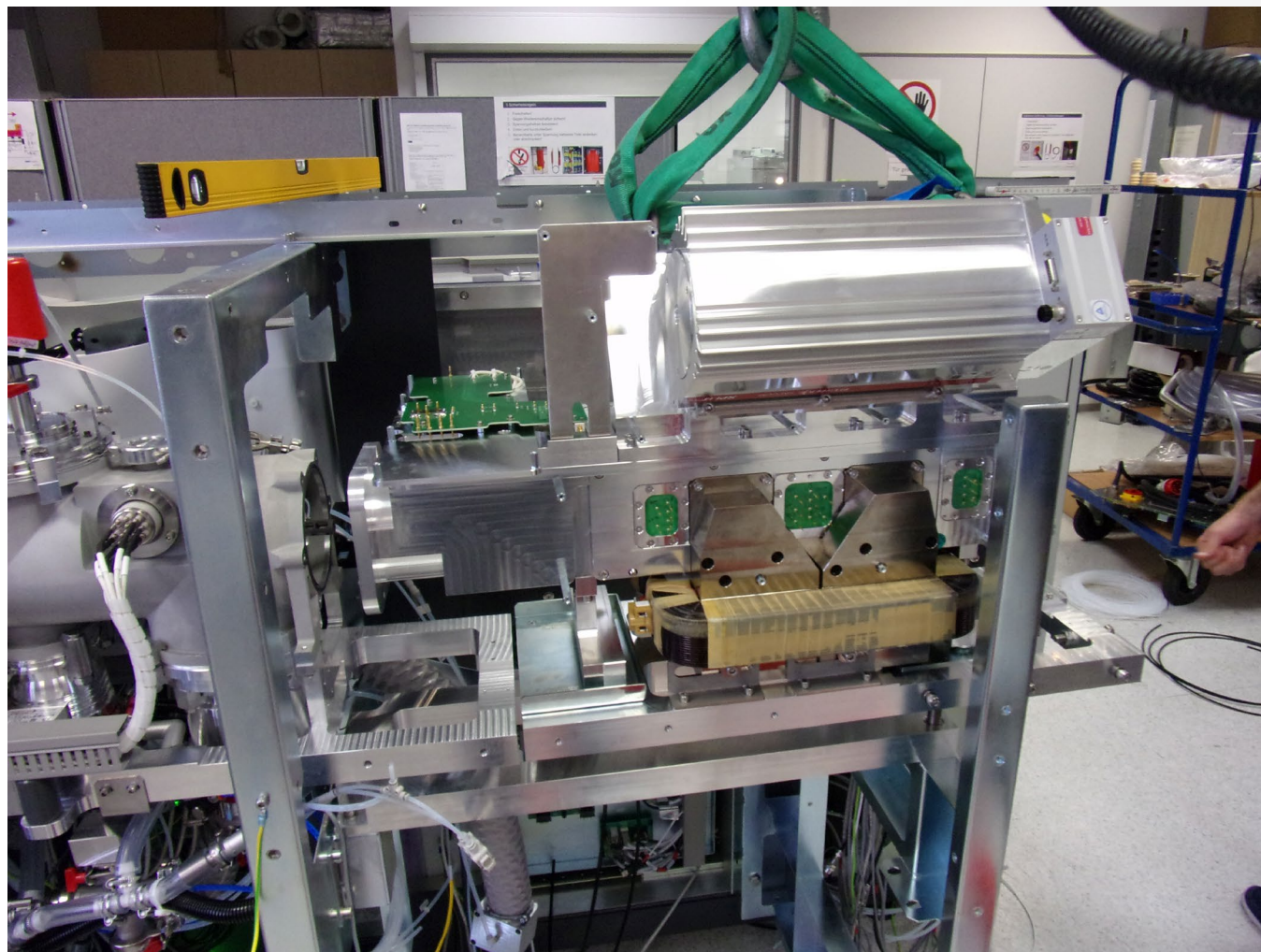
Preparing to install the MS/MS Option



Preparing to install the MS/MS option to the Neoma

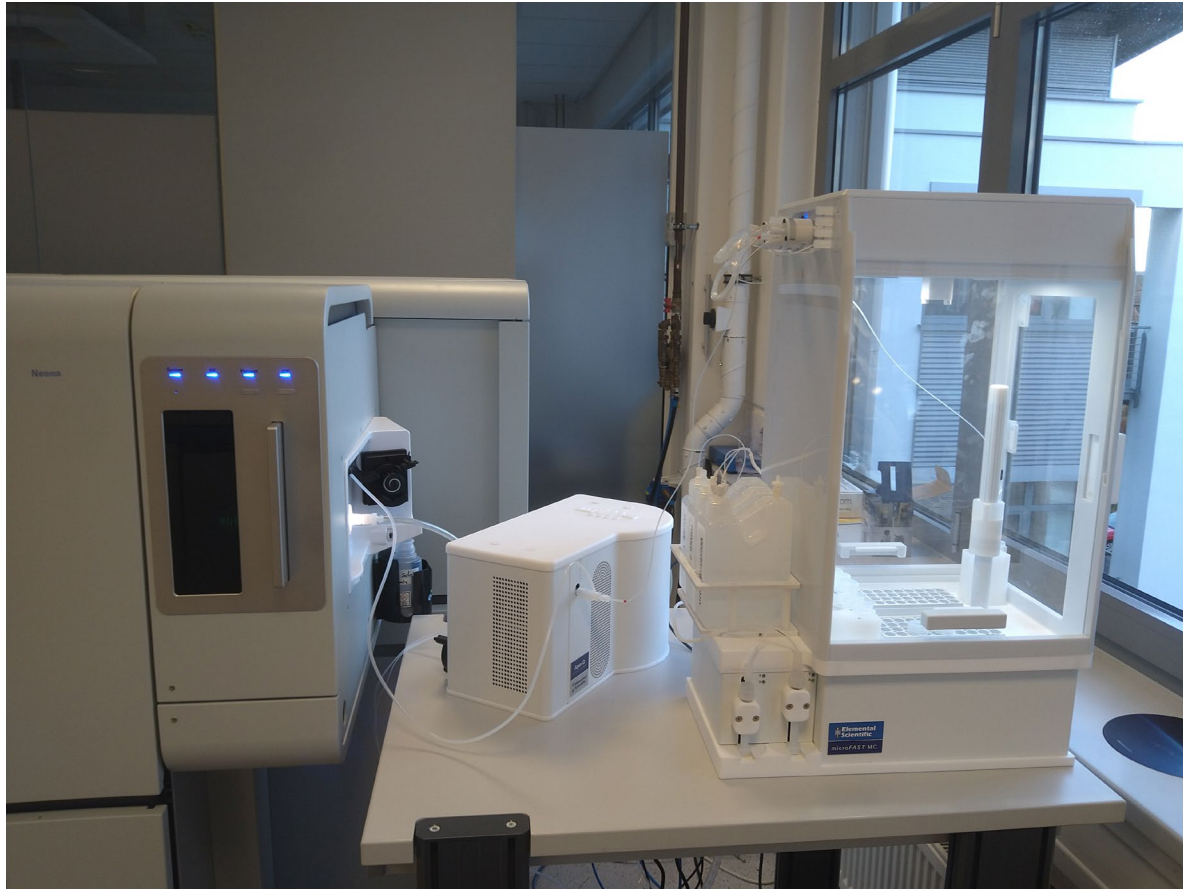


Adding the MS/MS option to the Neoma



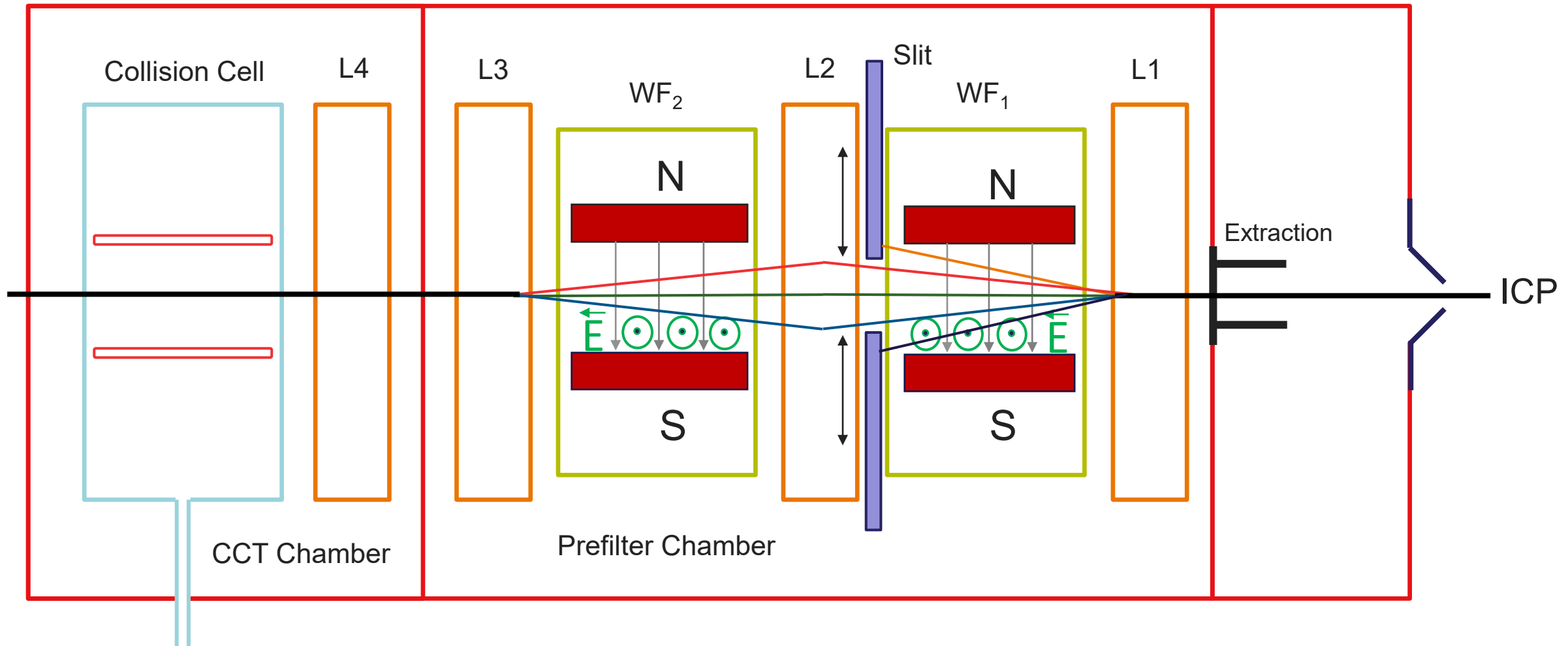
Neoma MS/MS

Instrument installed in the applications lab in Bremen



Neoma MS/MS Option

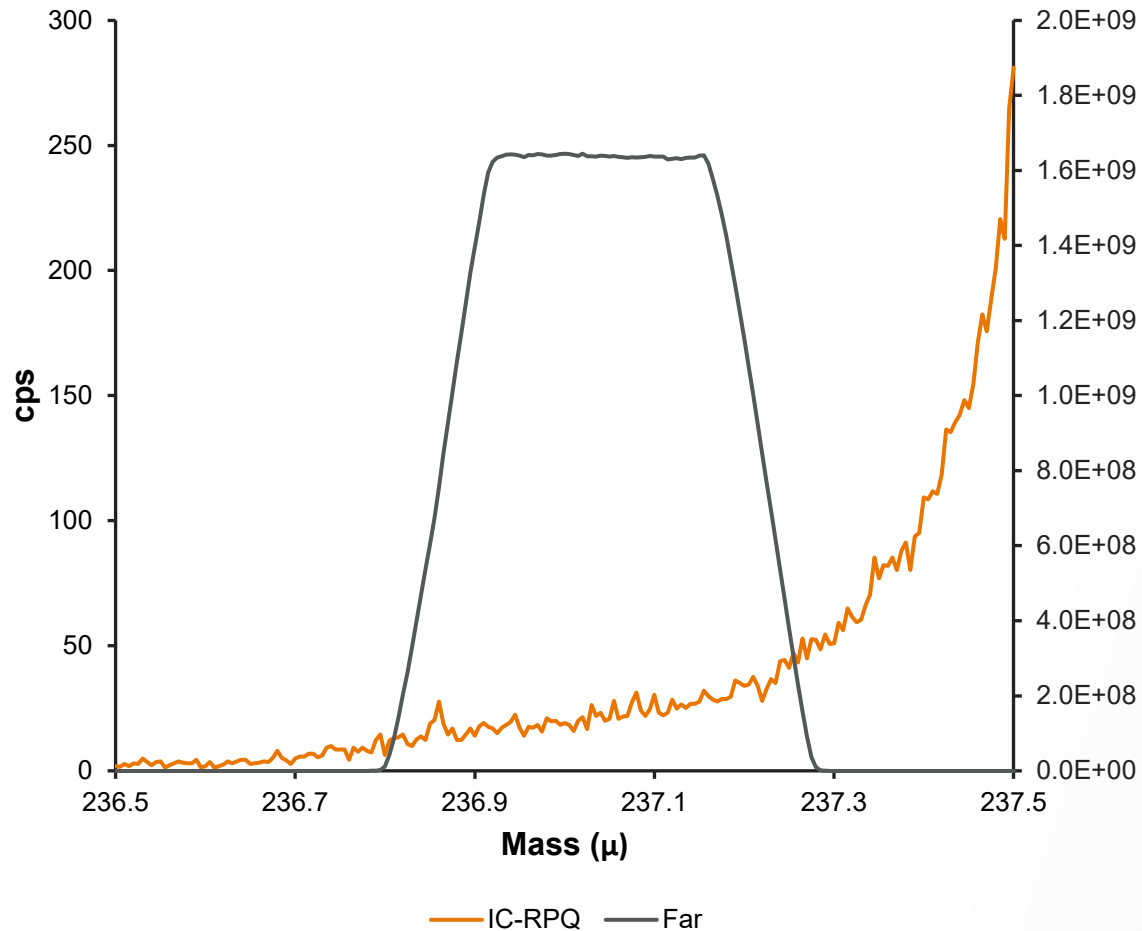
Based on prototype module developed on Thermo Scientific™ Vienna MC-ICP-MS/MS¹



1. Craig, G.; Wehrs, H.; Bevan, D. G.; Pfeifer, M.; Lewis, J.; Coath, C. D.; Elliott, T.; Huang, C.; Lloyd, N. S.; Schwieters, J. B. Project Vienna: A Novel Precell Mass Filter for Collision/Reaction Cell MC-ICPMS/MS. *Anal. Chem.* **2021**, 93 (30), 10519–10527.

Neoma MS/MS – Abundance Sensitivity

Neoma MS/MS removes $^{40}\text{Ar}^+$ early in the mass spectrometer.



- One of the earliest applications of triple quadrupole ICP-MS/MS was to measure ultralow $^{236}\text{U}/^{238}\text{U}$ ratios due to their excellent abundance sensitivity¹.
- Abundance sensitivity measured at 237.05
 - SEM Yield > 91%
 - $^{238}\text{U} = 1.64 \times 10^9$ cps (26.2 V, $10^{11} \Omega$)
 - 237.05 = 21 cps
- Abundance sensitivity < 0.013 ppm (13 ppb)
- Equivalent to specification on Thermo Scientific Triton Series™ TIMS
- Specification of Neoma MC-ICP-MS is only 0.5 ppm.

1. Tanimizu, M.; Sugiyama, N.; Ponzevera, E.; Bayon, G. Determination of Ultra-Low $^{236}\text{U}/^{238}\text{U}$ Isotope Ratios by Tandem Quadrupole ICP-MS/MS. *J. Anal. At. Spectrom.* **2013**, *28*, 1372–1376.

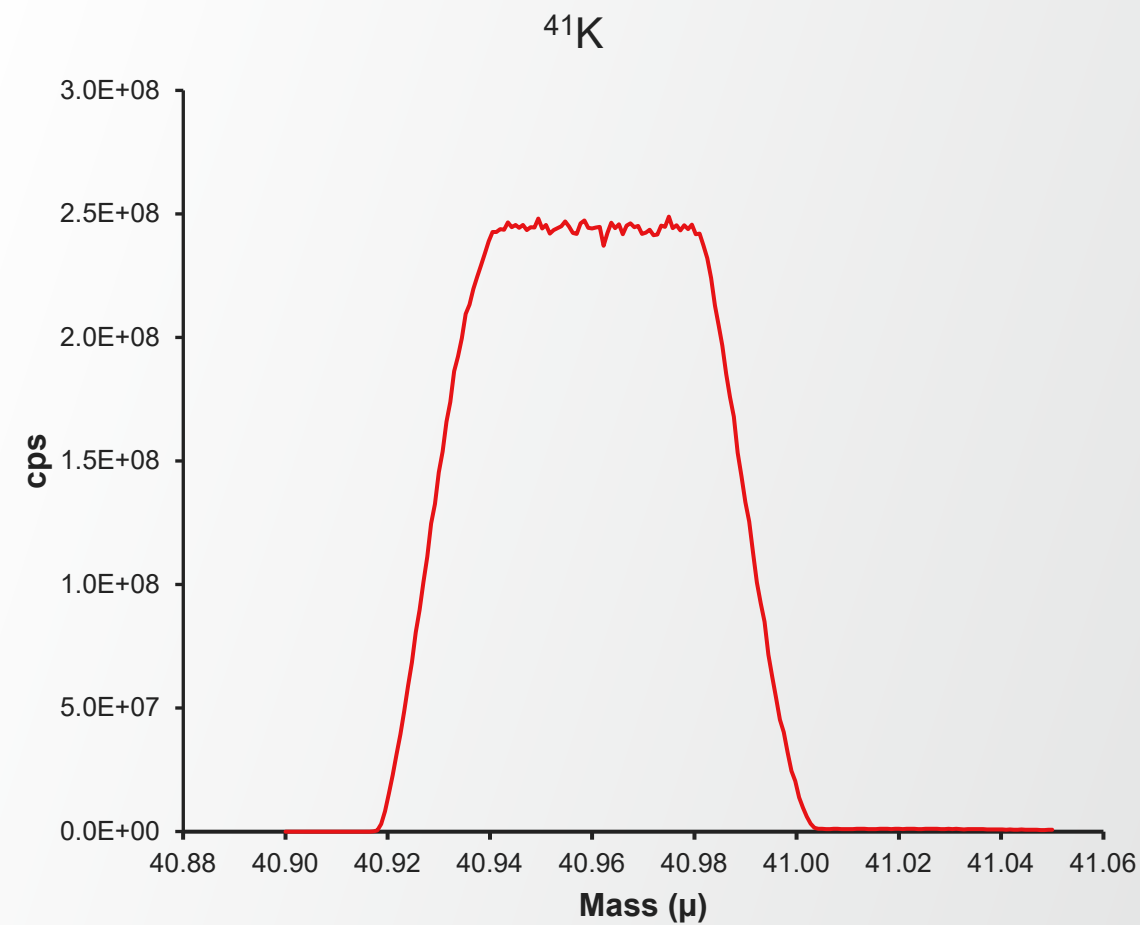
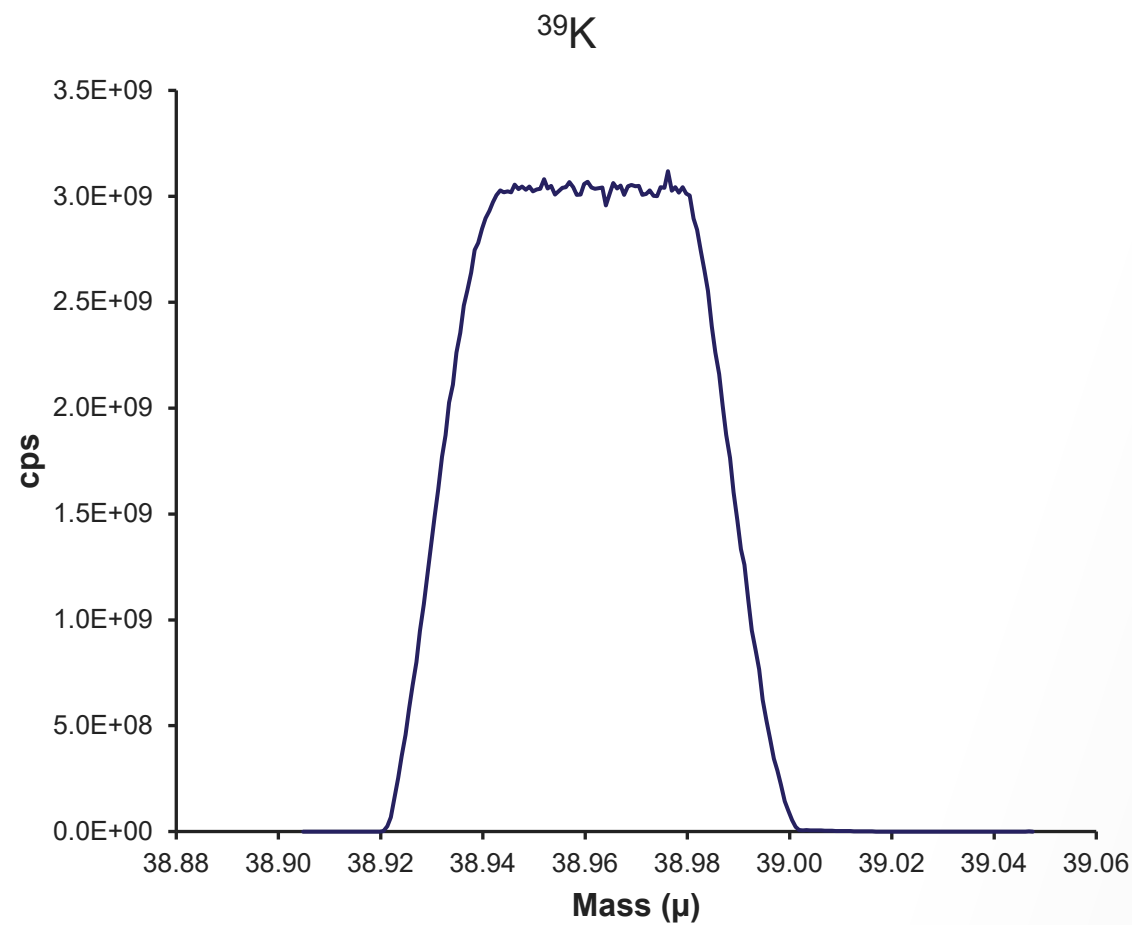
- For K and Ca we cannot prevent $^{40}\text{Ar}^+$ entering the collision/reaction cell.
- Instead of using the pre-cell mass filter, H_2 and He used to neutralize $^{40}\text{Ar}^+$ and $^{40}\text{ArH}^+$.
- K sensitivity significantly improved when compared to using resolution (XHR option) to separate $^{41}\text{K}^+$ from $^{40}\text{ArH}^+$.

[illegible]

Neoma MS/MS: low-level K with H₂ and He



K mass scans, 100 ng/g K, flow rate 50μL/min. 5.0mL/min H₂ and 1.5 mL/min He. ⁴⁰ArH⁺ interferent on ⁴¹K⁺ is eliminated.



Ratio No.	Delta No.	³⁹ K	⁴¹ K	⁴¹ K/ ³⁹ K	SE	δ ⁴¹ K	SE
1		1.21E+09	9.71E+07	8.026E-02	1.268E-06		
2	1	1.21E+09	9.72E+07	8.027E-02	1.915E-06	0.023	0.024
3		1.21E+09	9.72E+07	8.026E-02	1.577E-06		
4	2	1.21E+09	9.72E+07	8.026E-02	1.252E-06	-0.019	0.016
5		1.21E+09	9.71E+07	8.026E-02	1.170E-06		
6	3	1.20E+09	9.66E+07	8.027E-02	1.141E-06	0.028	0.014
7		1.20E+09	9.65E+07	8.027E-02	1.432E-06		
8	4	1.20E+09	9.67E+07	8.027E-02	1.325E-06	-0.031	0.017
9		1.20E+09	9.57E+07	8.022E-02	4.499E-05		
10	5	1.19E+09	9.57E+07	8.027E-02	7.804E-07	0.038	0.010
11		1.19E+09	9.56E+07	8.027E-02	1.134E-06		
12	6	1.19E+09	9.56E+07	8.027E-02	1.245E-06	-0.017	0.016
13		1.19E+09	9.53E+07	8.028E-02	1.163E-06		
14	7	1.18E+09	9.50E+07	8.028E-02	9.693E-07	0.038	0.012
15		1.17E+09	9.43E+07	8.027E-02	1.260E-06		
16	8	1.18E+09	9.44E+07	8.027E-02	1.102E-06	-0.008	0.014
17		1.18E+09	9.45E+07	8.028E-02	1.299E-06		
18	9	1.18E+09	9.45E+07	8.027E-02	1.100E-06	-0.036	0.014
19		1.18E+09	9.45E+07	8.027E-02	9.635E-07		
20	10	1.17E+09	9.42E+07	8.028E-02	9.220E-07	0.046	0.011
21		1.17E+09	9.40E+07	8.027E-02	2.672E-06		
22	11	1.17E+09	9.43E+07	8.027E-02	8.787E-07	-0.033	0.011
23		1.16E+09	9.34E+07	8.028E-02	9.788E-07		
24	12	1.17E+09	9.35E+07	8.028E-02	1.133E-06	0.002	0.014
25		1.17E+09	9.36E+07	8.028E-02	8.861E-07		
		³⁹ K	⁴¹ K	⁴¹ K/ ³⁹ K	SE	δ ⁴¹ K	SE
	Mean	1.19E+09	9.53E+07	8.027E-02	2.982E-06	0.003	0.014
	SD			1.196E-05		0.031	

Method

- 25ng/g SRM3141a K SSB against itself
- ESI™ Apex Omega™ desolvating nebulizer system.
- ESI *micro*FAST™ MC autosampler (dual loop with sample injection)
- Jet Cones
- 3-minute measurement (45 x 4s)
- 0.15 mL of solution
- 12 replicates
- Blank corrected
- 3.5mL H₂ & 2.5 mL/min He

Result

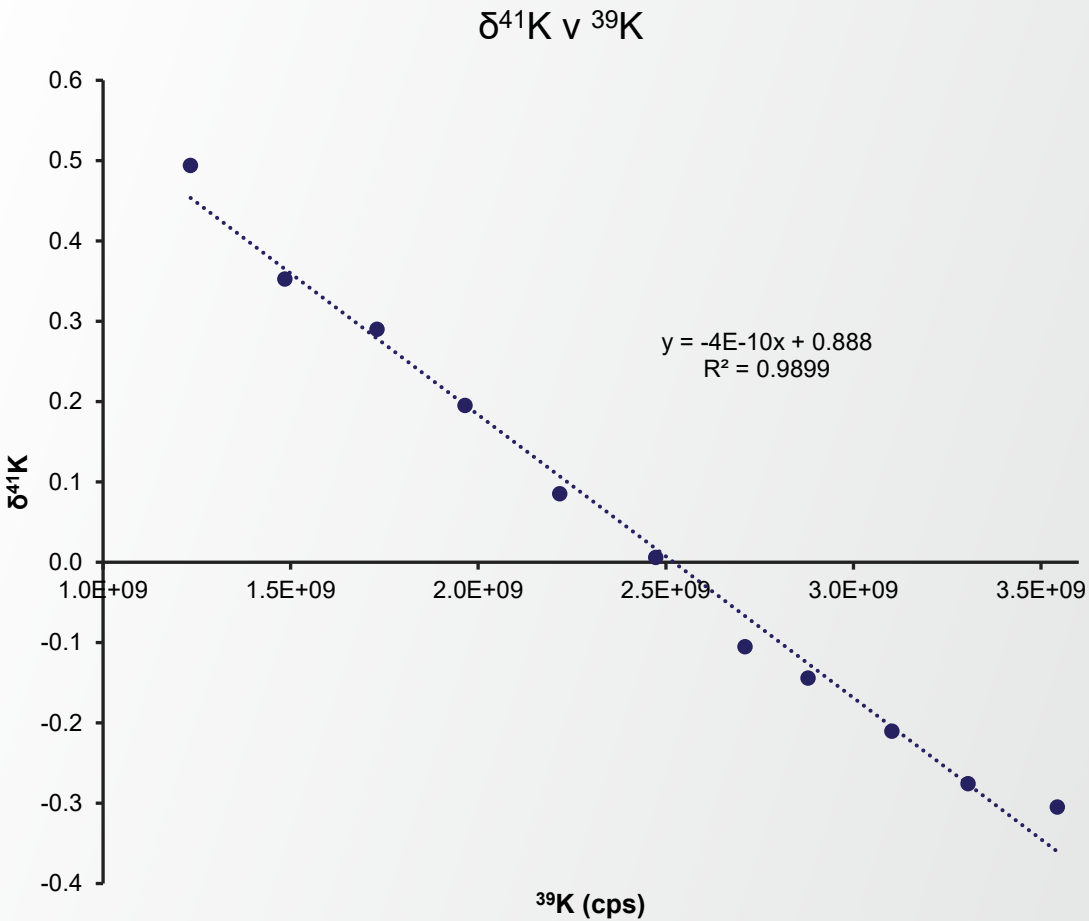
- δ⁴¹K = 0.003 ± 0.031 ‰ (1SD, n=12)
- Sensitivity > 1600 V/ppm

δ⁴¹K –sample-standard signal matching



Signal matching is vital for accurate δ⁴¹K, microFAST MC can be used to make this easy. Each 1% of difference changes δ⁴¹K by 0.01 ‰.

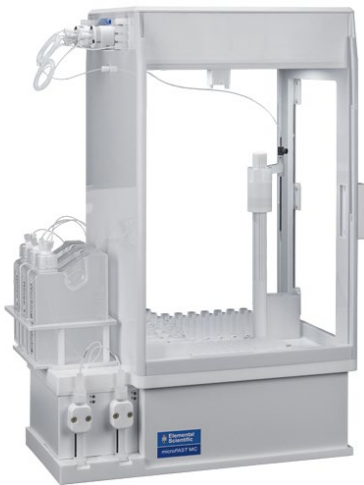
	³⁹ K (cps)	⁴¹ K (cps)	⁴¹ K/ ³⁹ K	2SE	δ ⁴¹ K _{SRM3141a}	2SE
50 μL/min	1.23E+09	9.55E+07	0.07745	1.88E-06	0.494	0.024
60 μL/min	1.48E+09	1.15E+08	0.07743	2.32E-06	0.353	0.030
70 μL/min	1.73E+09	1.34E+08	0.07742	1.82E-06	0.290	0.024
80 μL/min	1.96E+09	1.52E+08	0.07741	1.65E-06	0.195	0.021
90 μL/min	2.22E+09	1.72E+08	0.07740	1.51E-06	0.085	0.020
100 μL/min	2.47E+09	1.91E+08	0.07740	1.48E-06	0.006	0.019
110 μL/min	2.71E+09	2.10E+08	0.07739	1.68E-06	-0.105	0.022
120 μL/min	2.88E+09	2.23E+08	0.07739	1.50E-06	-0.144	0.019
130 μL/min	3.10E+09	2.40E+08	0.07739	1.29E-06	-0.210	0.017
140 μL/min	3.31E+09	2.56E+08	0.07738	1.18E-06	-0.275	0.015
150 μL/min	3.54E+09	2.74E+08	0.07738	2.04E-06	-0.305	0.026



ESI™ microFAST MC™ Dual Loop Autosampler



Driven with Qtegra ISDS for Neoma MC-ICP-MS



- Used for small volume samples of between 5-1000 µL/min
- Dual loop for high throughput and reduced carryover
- Stable injection profiles for precise isotope ratios
- *microFAST MC* was extremely difficult to use with previous generation MC-ICP-MS.
- Plugin for Qtegra ISDS makes using this autosampler extremely easy.
- Select total sample amount and sample injection rate in the sample list.

Sample List																			
	Label	Status	Comment	Sample Type	Peak Center	Gain	Electronic Offset	Evaluate	Standard	Rack Number	Vial Numbers	Sample Loading Volume	Sample Injection Rate						
1	Blank	●	<Comment>	QC						0	7	650	100						
2	Blank	●	<Comment>	BLK						0	7	650	100						
3	SRM3141a	●	<Comment>	STD						0	4	650	100						
4	SRM9996b	●	<Comment>	SMP						0	3	650	100						
5	SRM3141a	●	<Comment>	STD						0	4	650	100						
6	SRM9996b	●	<Comment>	SMP						0	3	650	100						
7	SRM3141a	●	<Comment>	STD						0	4	650	100						
8	SRM9996b	●	<Comment>	SMP						0	3	650	100						
9	SRM3141a	●	<Comment>	STD						0	4	650	100						
10	SRM9996b	●	<Comment>	SMP						0	3	650	100						
11	SRM3141a	●	<Comment>	STD						0	4	650	100						
12	SRM9996b	●	<Comment>	SMP						0	3	650	100						
13	SRM3141a	●	<Comment>	STD						0	4	650	100						
14	SRM9996b	●	<Comment>	SMP						0	3	650	100						

Standard – Sample Signal Matching

Moynier *et al.* 2021 *Chem. Geo.*, **571**, 120144

- Literature shows the importance of matching standard and sample signal for accurate $\delta^{41}\text{K}$ analysis
- Neoma (and Neoma MSMS) in combination with the ESI *microFAST* MC can signal match by varying uptake rate.

Sample List																										
	Label	▼ ▴	Status	▼ ▴	Comment	▼ ▴	Sample Type	▼ ▴	Peak Center	▼ ▴	Gain	▼ ▴	Electronic Offset	▼ ▴	Evaluate	▼ ▴	Standard	▼ ▴	Rack Number	▼ ▴	Vial Numbers	▼ ▴	Sample Loading Volume	▼ ▴	Sample Injection Rate	▼ ▴
1	Do not use		●		100ppb K in 0.5		BLK		☐		☐		☐		☐					0		5		650		100
2	Do not use		●		100ppb K in 0.5		BLK		☐		☐		☐		☐					0		5		650		100
3	Blank		●		100ppb K in 0.5		BLK		☐		☐		☐		☒		SRM3141a			0		5		650		100
4	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
5	SRM996b		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		9		650		114
6	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
7	SRM996b		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		9		650		114
8	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
9	SRM996b		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		9		650		114
10	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
11	SRM996b		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		9		650		114
12	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
13	SRM996b		●		100ppb K in 0.5		SMP		☐		☐		☐		☐					0		9		650		114
14	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
15	Blank		●		100ppb K in 0.5		BLK		☐		☐		☐		☒					0		5		650		100
16	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
17	SRM985		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		10		650		93
18	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
19	SRM985		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		10		650		93
20	SRM3141a		●		100ppb K in 0.5		STD		☐		☐		☐		☒		SRM3141a			0		7		650		100
21	SRM985		●		100ppb K in 0.5		SMP		☐		☐		☐		☒					0		10		650		93

LA-MC-ICP-MS: Neoma MC-ICP-MS/MS + NWR193 LA



In-situ B

Laser Conditions

- 6 J/cm² Fluence
- 13 Hz repetition rate
- 100 µm circle spot size
- Jet Interface
- 0.750 L/min He
- 4 mL/min N₂

Reference Materials

NIST SRM610

JCt-1

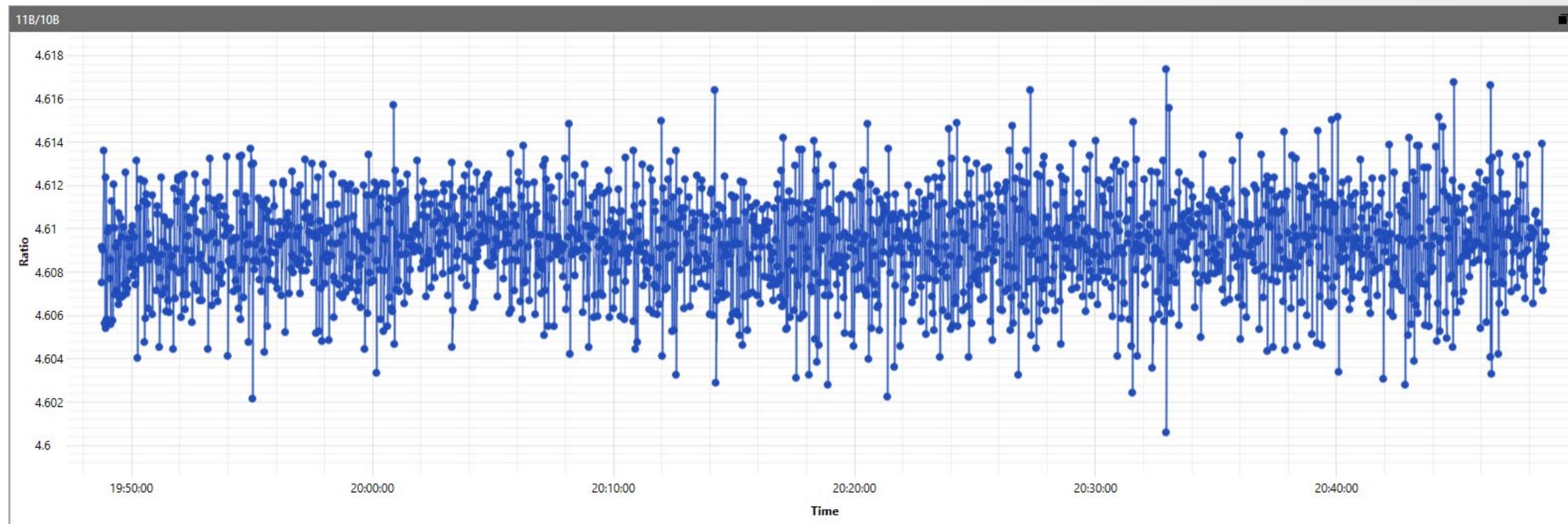
JCp-1



Cup	L5	L4	L3	L2	L1	C	H1	H2	H3	H4	H5
10B	⁹ Be					¹⁰ B					¹¹ B
11B	¹⁰ B					¹¹ B					¹² C
10.5	¹⁰ B								¹¹ B		

Boron

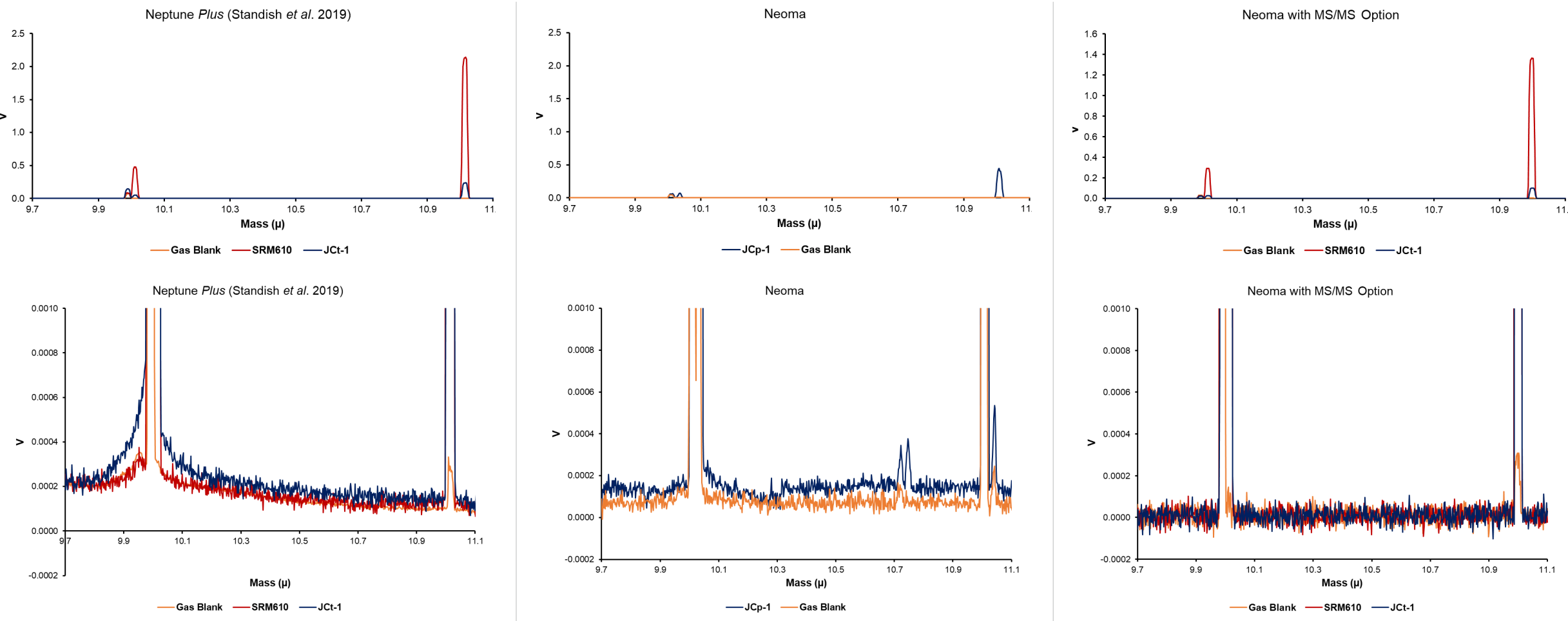
50ppb Boron, Jet Interface, 1 hr stability, **drift = 12 ppm.**



B Baseline – Ablating Carbonates

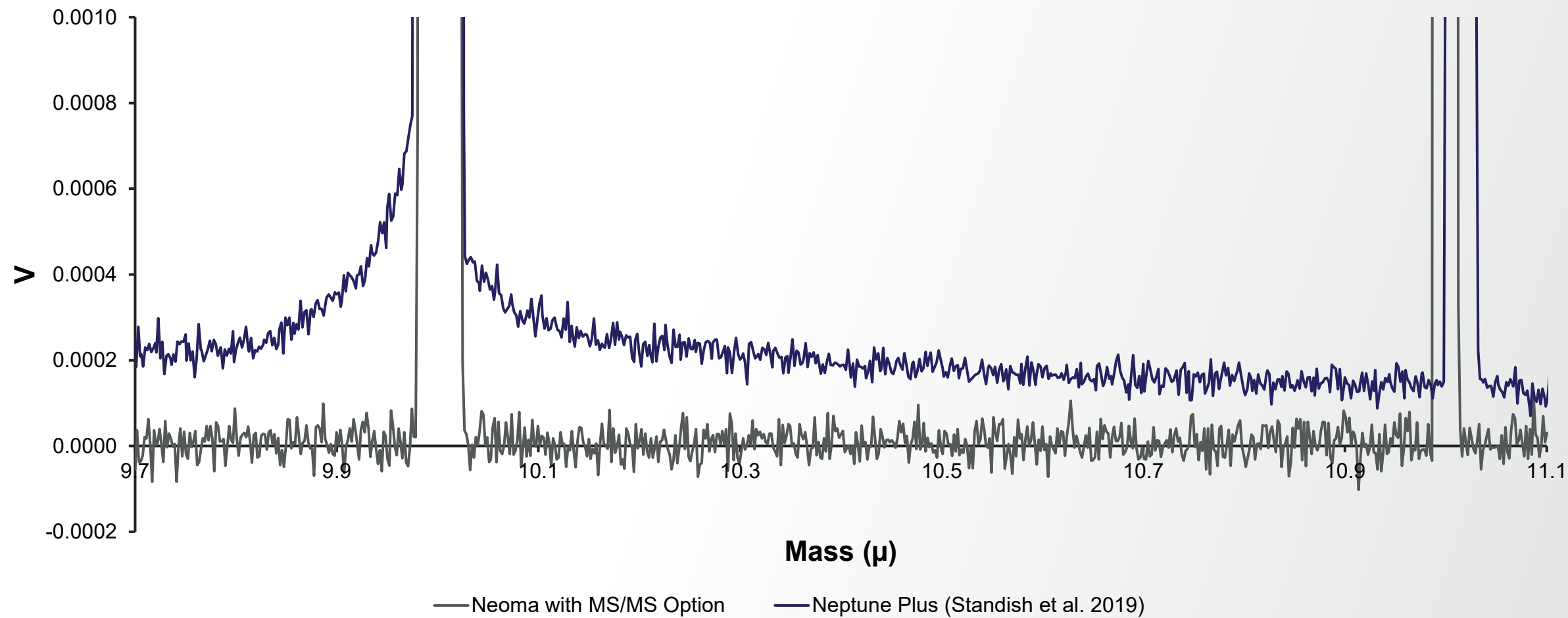


Neptune *Plus* v. Neoma v. Neoma with MS/MS Option



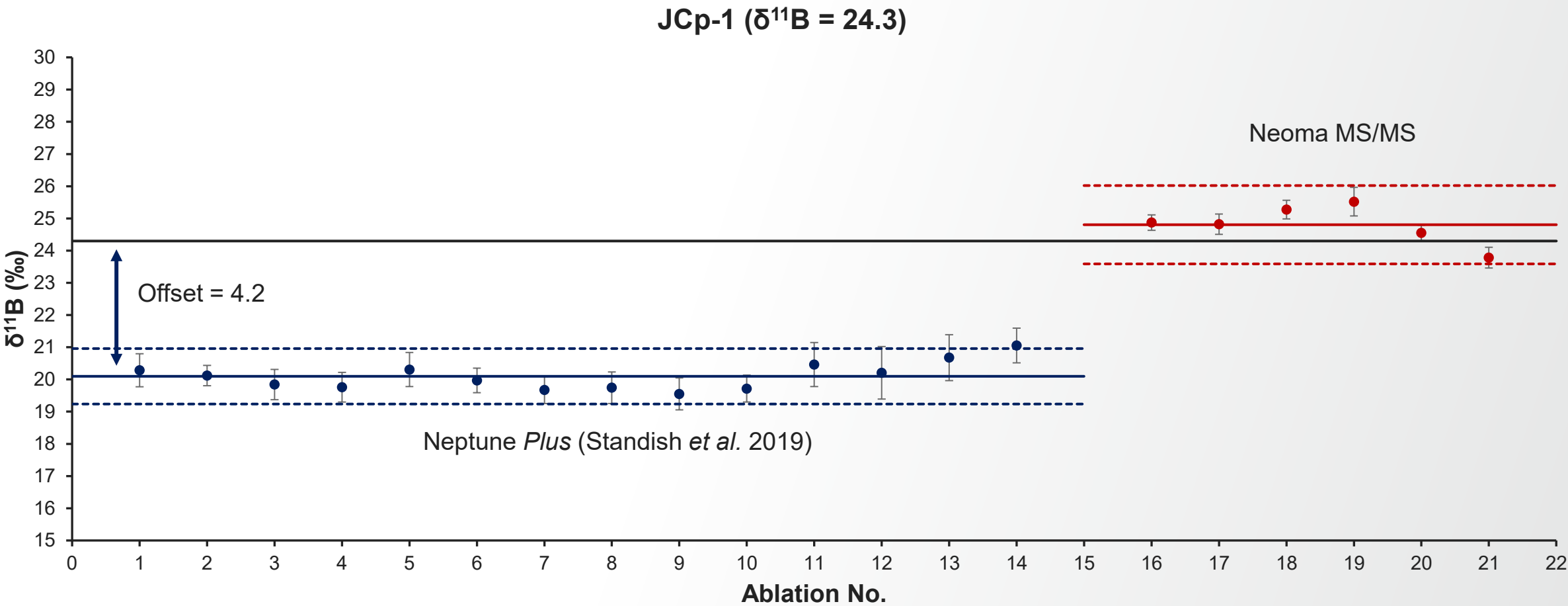
B Baseline

Neoma with MS/MS Option eliminates the rising baseline seen on the Neptune Series MC-ICP-MS



B: JCp-1

No offset in B isotope ratios for Neoma MS/MS



Conclusion

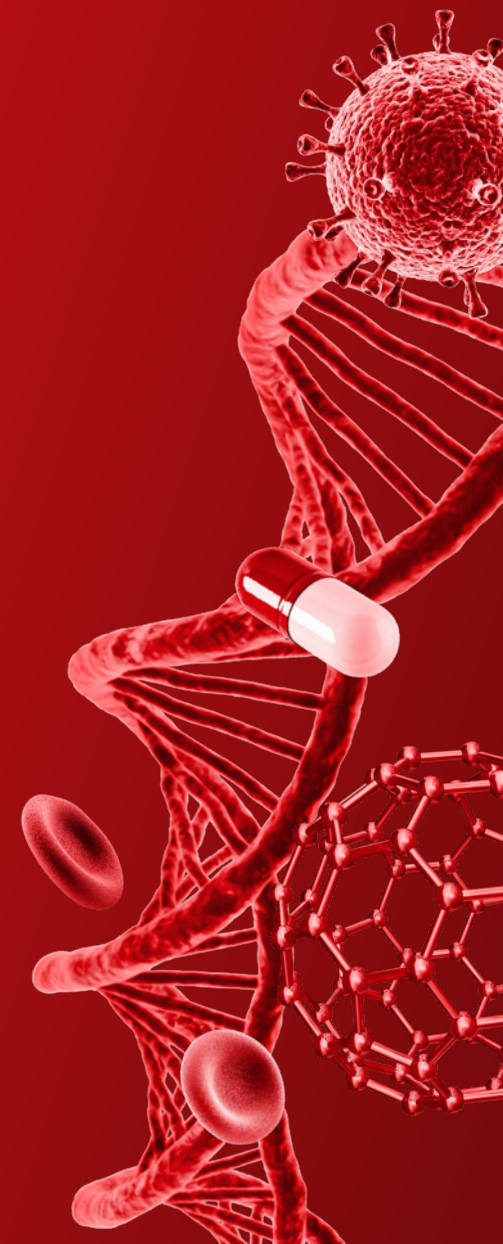
Thermo Scientific™ Neoma™ MC-ICP-MS with MS/MS Option

- ‘Triple Quad’ applications with MC-ICP-MS precision
- Unique pre-cell mass filter and collision/reaction cell design.
- Latest Thermo Scientific Neoma MC-ICP-MS platform.
 - Enhanced detector array.
 - Thermo Scientific Qtegra ISDS™ software.
 - Robust iCAP Qnova™ Series ICP.
 - Comprehensive data evaluation including transient signal analysis.
 - All new electronics and enhanced vacuum system.
- Wide array of potential applications.

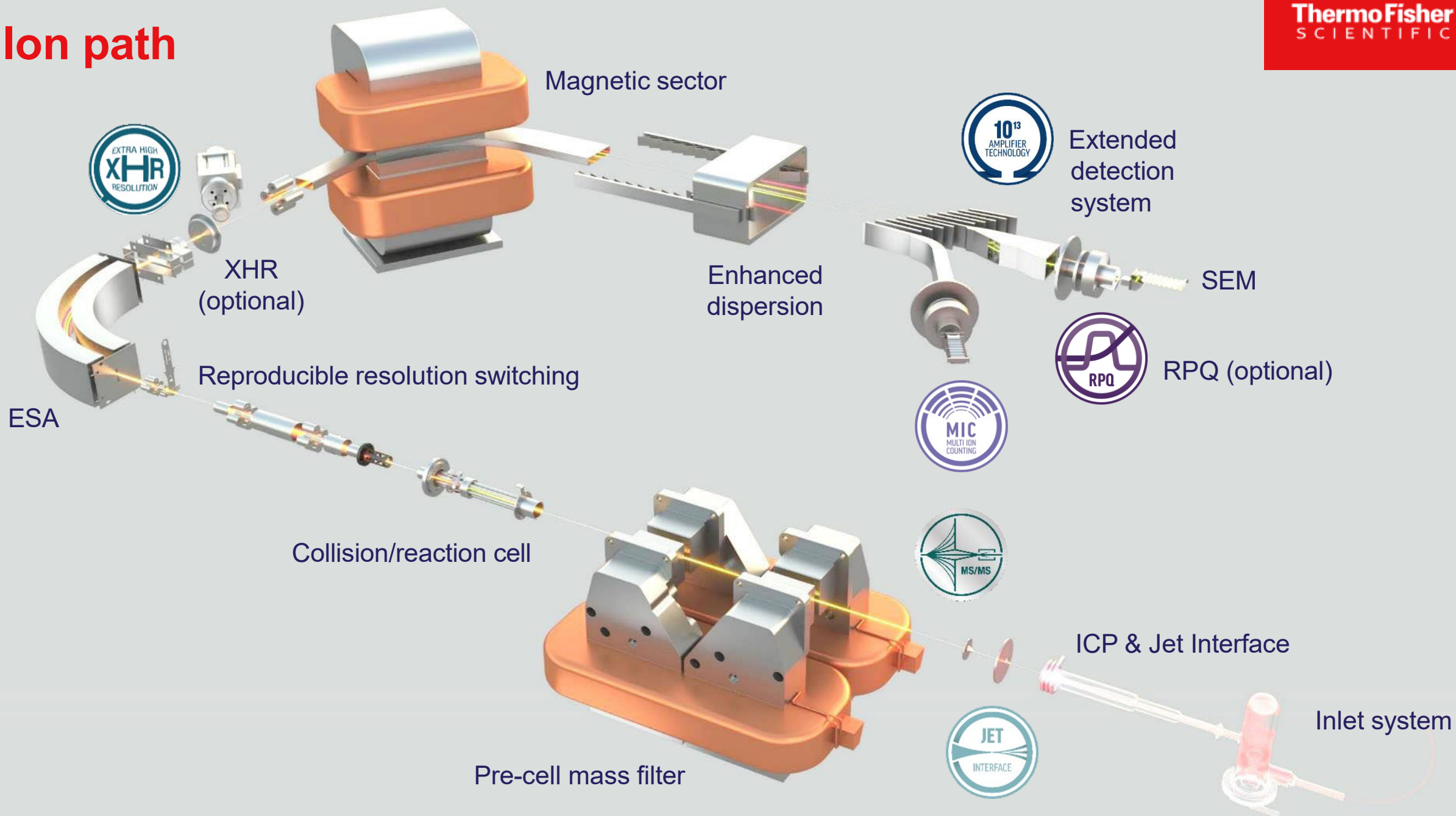


Thank you

Questions?



Ion path



MS/MS technology



- Plain collision-reaction cell
 - No pre-cell mass filter: everything enters the cell
 - Many unwanted collisions and reactions take place
 - Can only work with specific gases
- CRC with MS/MS technology
 - Pre-cell mass filter: allows a selected mass range to enter the cell, rest of the masses do not enter the cell
 - No unwanted collisions and reactions in the cell
 - Can work with more gases
 - Besides classical systems (Ca, K), it can also do more complicated ones (Rb/Sr, Cr, Ti, Si, ...)
 - Excellent abundance sensitivity

