RV *INVESTIGATOR*

HYDROCHEMISTRY DATA PROCESSING REPORT

Voyage:	IN2026_V02
Chief Scientist	Prof. Nicole Jones
Voyage title:	Quantifying the fine scale ocean dynamics of the Ningaloo Coast
Report compiled by:	Kurt Debruille, Julie Janssens, Merinda McMahon, and Stephen Tibben

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Executive Summary

Voyage Objectives

1. **Develop and test novel techniques to derive, with quantified uncertainty, oceanic submesoscale currents (0.1-10 km) from remotely sensed sea surface height (SSH) and/or sea surface temperature (SST) observations.**

   Our understanding of submesoscale features (at spatio-temporal scales ~0.1–10 km and 0.1–10 d) has been limited by our ability to measure ocean currents at these scales. New Earth observing satellites can elucidate submesoscale features, as they now have sufficient resolution and map wide swaths of ocean tracers. A new low-altitude camera system will provide even finer resolution surface current information. Inversion techniques will be developed and tested to estimate ocean currents at unprecedented resolution.

2. **Optimise data assimilation techniques for improved ocean reanalysis and forecasts.**

   The benefits of ingesting newly available remotely sensed data, such as SWOT altimetry into data assimilation numerical models of ocean circulation is untested. We will create an important data set for the development and validation of data assimilating models, leading to improved ocean forecasts.

3. **Investigate lateral and vertical transport processes associated with oceanic submesoscale currents and their relation to turbulent mixing within the surface mixing layer.**

   As the submesoscale is unresolved in operational and global climate models, their effect must be parameterised. The surface mixing layer's response to submesoscale processes and the interplay with near-inertial and Ekman dynamics are also poorly understood. The novel observations proposed in this study will determine the relationship between mesoscale processes, submesoscale processes and vertical mixing, creating the process understanding required for parameterisation.

4. **Quantify the fluxes of nutrients to Ningaloo Reef.**

   Limited studies have demonstrated that eddies and upwelling contribute to nutrient inputs in the nearshore environment of Ningaloo Reef. This study will quantify the role of submesoscale features in the transport of nutrients to Ningaloo Reef, with applications to coastal environments elsewhere.

5. **Characterise the submesoscale current fields on the Ningaloo Coast and quantify spatial variability of eddy properties including hotspots of submesoscale activity that control ocean transport.**

   Submesoscale features play a key role in the horizontal dispersion of ocean-borne material, including heat, nutrients, coral larvae, pollutants like oil and plastics, and floating objects. They are also responsible for some of the largest observed surface currents on the Ningaloo Coast.

Combining ocean circulation models with *in-situ* and remotely sensed observations will allow us to quantify the geographical and seasonal variability of submesoscale currents.

General Hydrochemistry Information

For this voyage, CTD samples were collected and analysed for nutrients, dissolved oxygen, and salinity by the on-board Hydrochemistry team. Discrete underway nutrient samples were also measured. Underway nutrients were also continuously analysed during ADCP and Triaxus transects using a Seal AA100. Additionally, Thermosalinograph (TSG) samples were collected throughout the voyage, with on-board measurements of their salinity used to calibrate the ship's underway system.

Please cite the following manuscript when reporting or publishing data for silicate, phosphate, nitrate+nitrite (NO_x) and nitrite:

Rees, C., L. Pender, K. Sherrin, C. Schwanger, P. Hughes, S. Tibben, A. Marouchos, and M. Rayner. (2018) "*Methods for reproducible shipboard SFA nutrient measurement using RMNS and automated data processing*."

Limnol. Oceanogr: Methods, 17(1): pp. 25-41.

DOI: 10.1002/lom3.10294

If publishing ammonium data, please cite the following:

Rees, C., Janssens, J., Sherrin, K., Hughes, P., Tibben, S., McMahon, M., McDonald, J., Camac, A., Schwanger, C. and Marouchos, A., (2021*) "Method for Reproducible Shipboard Segmented Flow Analysis Ammonium Measurement Using an In-House Reference Material for Quality Control."*

Frontiers in Marine Science, 8.

DOI: 10.3389/fmars.2021.581901

The final hydrology dataset, data processing report, analytical methods, related log sheets and processing notes can be obtained from the CSIRO data centre. Please visit CSIRO data trawler, should there be any inquiries on hydrology data please contact CSIRO data centre at NCMI_DataLibrarians@csiro.au.

Itinerary and Voyage track

Table 1: Voyage itinerary

	Depart	**Arrive**
Port	Fremantle	Fremantle
Date	17/03/2026	17/04/2026
Time	0800	0800

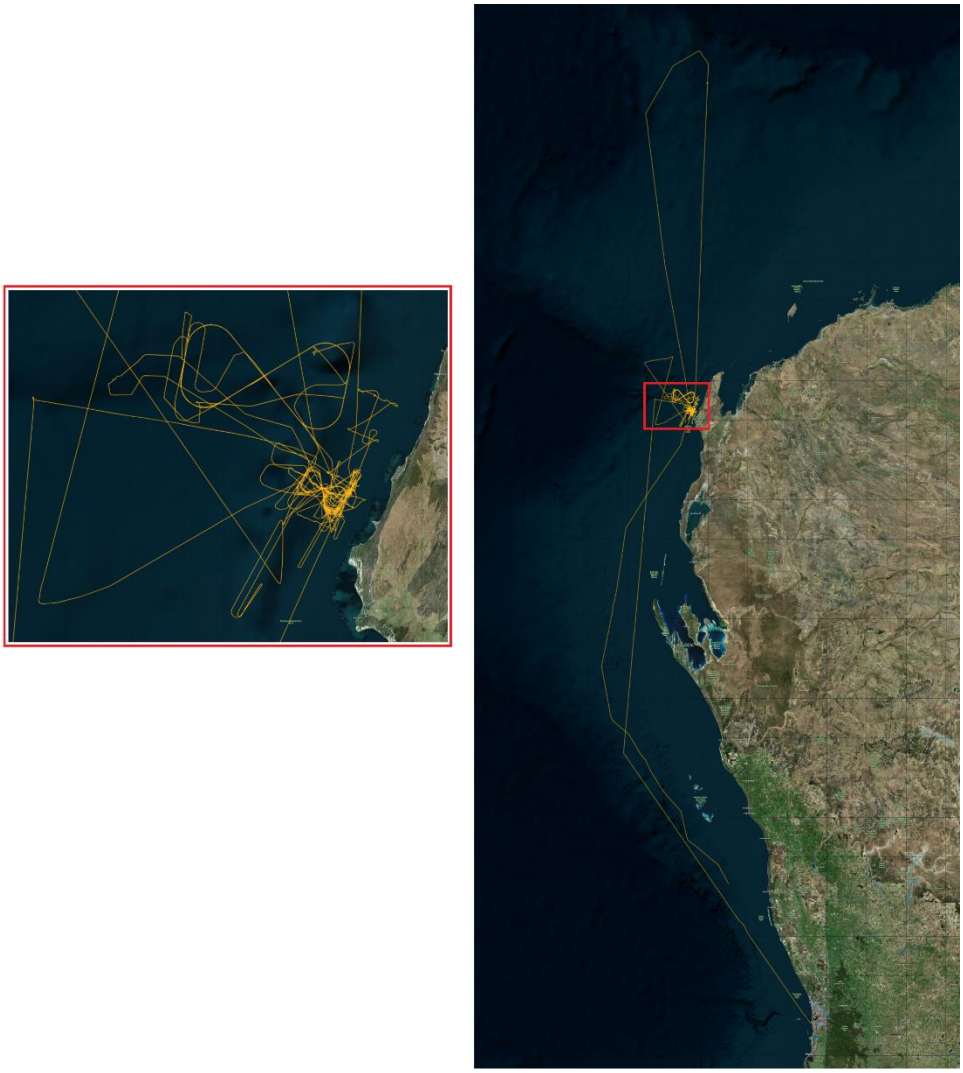

Figure 1. Voyage map

Key personnel list

Table 2: Key Personnel list

Name	Role	Organisation
Prof. Nicole Jones	Chief Scientist	UWA
Max McGuire	Voyage Manager	CSIRO
Kurt Debruille	Hydrochemist	CSIRO
Julie Janssens	Hydrochemist	CSIRO
Merinda McMahon	Hydrochemist	CSIRO
Stephen Tibben	Hydrochemist	CSIRO

Sample Summary

Sample Type and Number Assayed

Table 3: Hydrochemistry sample type and analysis summary

Analysis	Instrument	Sample source/type	Number of samples
Nutrients	Seal AA500 / AA100	Conductivity-Temperature-Depth (CTD) Underway (UWY)	373 294
Salinity	Guidline Autosal	Conductivity-Temperature-Depth (CTD) Thermosalinograph (TSG)	223 32
Dissolved oxygen (DO)	Scripps automated titration	Conductivity-Temperature-Depth (CTD)	222

CTD sample (Conductivity, Temperature, Depth)

Table 4: CTD summary

Rosette type	36
Niskin Bottle size	12 L
Number of deployment	53
Number of deployment sampled for hydrochemistry analyses	37
CTD sampling order	Dissolved Oxygen (DO) ⟶ Nutrients ⟶ Salinity
Sample bottle	DO: 140 mL glass iodine determination flasks with glass stopper Nutrient: 50 mL HDPE with screw cap lids Salinity: 200 mL volume OSIL bottles made of type II glass (clear) with disposable plastic insert and plastic screw cap
Sample log	CTD deployment paper log sheet and CAP Deployment Log Editor version 1.4.5
Sampling personnel (hydrochemistry)	Kurt Debruille, Julie Janssens, Merinda McMahon, and Stephen Tibben
Sampling personnel (science party)	Bozena Wojtasiewicz, Tamara Schlosser, Thivin Abeywickrama, William Edge, Sina Pinter and Prashant Pujari

CTD 001 to 005, 007 to 017, 035 to 039, and 043 to 053 were sampled for DOs, salinities and nutrients. CTD 006 sampled for DO and salt only. CTD 024, 025, 027, 029, 030, and 034 were sampled for nutrients only. CTD 032 was sampled for nutrients and salts only. CTDs 015 to 023, 026, 028, 031, 033, 040, 041, and 042 were not sampled for hydrochemistry.

Underway sample (UWY)

Table 5: UWY summary

UWY source	Instrument clean seawater line supplying the pCO2 instrument in the underway laboratory. The line was cleaned with bleach in March 2026.
Sample bottle	Nutrient: 30 mL PP tube with screw cap lids Salinity: 200 mL volume OSIL bottles made of type II glass (clear) with crimp cap
Sample log	UWY Samples Event Logs (available on CSIRO data trawler)
Sampling personnel (hydrochemistry)	Kurt Debruille, Julie Janssens, Merinda McMahon, and Stephen Tibben
Sampling personnel (science party)	N/A

Data Processing Overview

The sample meta-data, measured bottle salinity results, dissolved oxygen assay results and the nutrient assay raw data are processed using the CSIRO-developed program HyPro. This processing generates the final hydrology dataset. An overview of this process is illustrated below (fig.2).

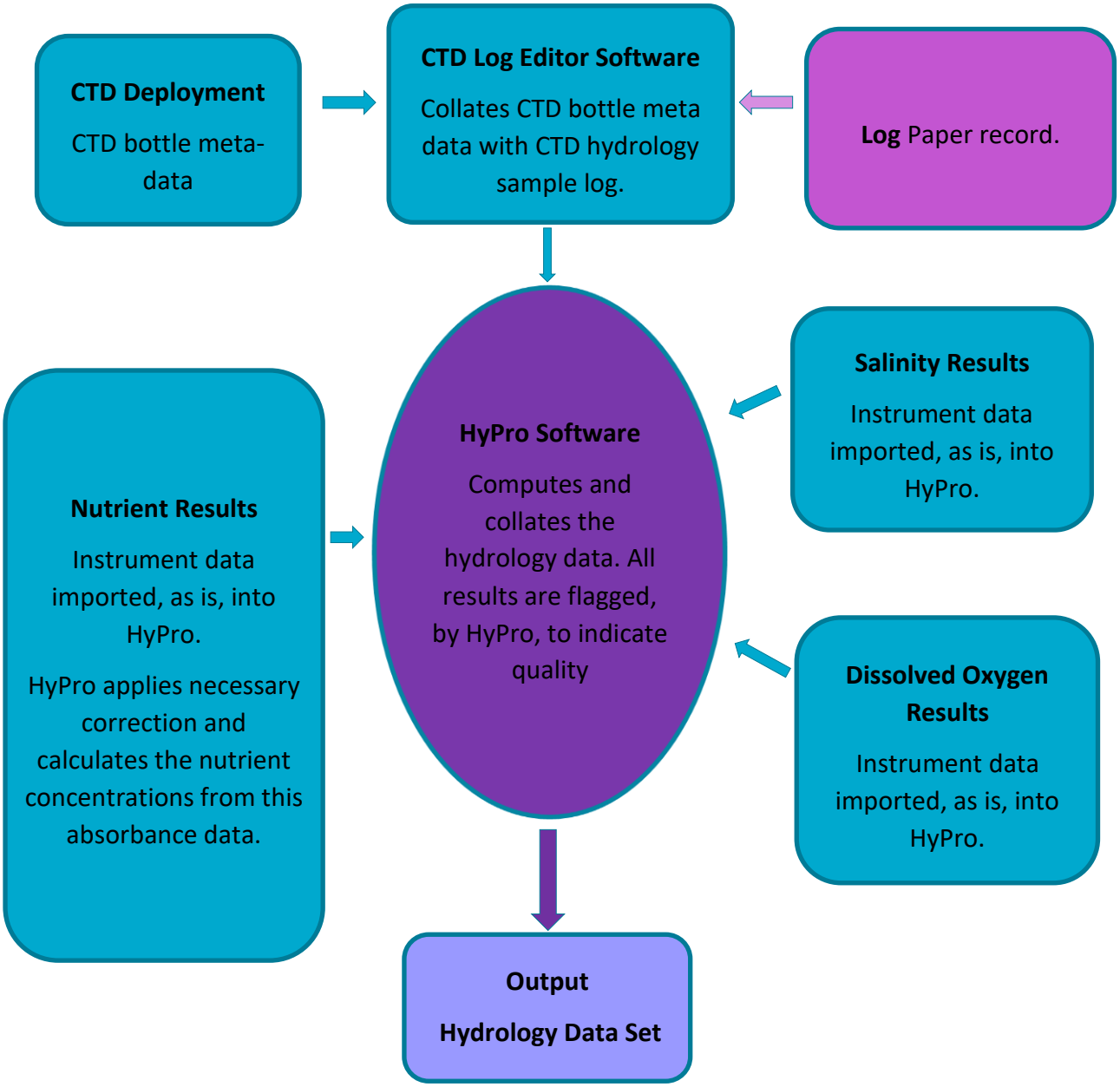

Figure 2. Conventional Hydrology Data Processing Flow Diagram.

Salinity

Salinity Measurement Parameters

Table 9. Salinity Measurement Parameters

Details	
HyPro Version	5.9
Instruments	Guildline Autosal Laboratory Salinometer 8400B – SN 72873. Bath temperature 24.0°C
Software	Ocean Scientific International Ltd (OSIL) Data Logger ver 1.2
Hydrochemistry Methods	Sampling: Salinity - WI_Sal_001, TSG – WI_Sal_004 Analysis: SOP 006
Accuracy	± 0.001 practical salinity units (PSU)
Reference Material	OSIL IAPSO – Batch P168, use by 01 December 2026, K_{15} = 0.99993
Sample Container	CTD: 200 mL volume OSIL bottles made of type II glass (clear) with disposable plastic insert and plastic screw cap. TSG: 200 mL volume type I (clear) borosilicate bottle with rubber liner lid and aluminium crimp cap.
Sample Storage	Stored in salinometer lab for minimum of 8 hrs for temperature equilibration before measurement
Analyst	Kurt Debruille, Julie Janssens, Merinda McMahon, and Stephen Tibben

Salinity Method

Salinity samples were measured on a Guildline Autosal 8400B, operated in accordance with the manufacturer's technical manual. The measured value is recorded with an OSIL data logger.

Practical salinity (S) is defined as the ratio (K_{15}) of the electrical conductivity of seawater measured at 15°C, 1 atm to that of a potassium chloride (KCl) solution of mass fraction 32.4356 x 10^{-3}.

Before each lot of sample measurements, the Autosal was calibrated with standard seawater (OSIL, IAPSO) with a known K_{15} ratio. A fresh bottle of OSIL standard is used for each calibration, and calibration is performed at least once per run.

Method summary: The salinity sample is collected in a 200 mL glass bottle. The bottle is rinsed three times with sample, then filled from the bottom, via a polytetrafluoroethylene (PTFE) straw, until overflowing. The bottle is removed from the straw, and the sample is decanted to allow a headspace of approximately 25 cm^3. A dry plastic insert is fitted, the bottle inverted and rinsed with ultra-pure water, wiped dry, capped and stored upside down until analysis. To measure, the salinometer cell is flushed three times with the sample and then measured after the third and fourth flush. The OSIL data logger software captures the conductivity ratio and calculates the practical salinity.

The output from the data logger is imported into HyPro and linked with the CTD deployment meta-data.

CTD Salinity vs Bottle Salinity

For this voyage, the difference between the unprocessed (uncorrected) CTD value and the measured bottle value is generally less than 0.02 PSU. The larger differences are often observed in shallow samples, where sudden changes in the thermohaline profile occurs. Occasionally, these discrepancies may also be attributed to mismatches between the CTD downcast and upcast profiles. CTD sensor data were recorded on the downcast, while bottle samples were collected on the upcast.

The unprocessed CTD values are adjusted (corrected) by DAP using the salinity bottle results. The corrected values are not reported in the hydrology set. Please refer to IN2026_V02 CTD data on CSIRO marlin metadata system for corrected sensor data.

OSIL Salinity Standard

For each salinity analysis conducted on this voyage, the instrument was calibrated with OSIL standard seawater, lot P168 (PSU = 34.997).

The mean measured value for the P168 OSIL standard seawater across the voyage was:

Mean = 34.9973 PSU SD = 0.0002 n = 10

Dissolved Oxygen

Dissolved Oxygen Measurement Parameters

Table 10. Dissolved oxygen measurement parameters.

Details	
HyPro Version	5.9
Instrument	Scripps Automated Photometric Oxygen System
Software	Scripps Institution of Oceanography (SIO)
Hydrochemistry Methods	Sampling: WI_DO_001 Analysis: SOP 005
Titrant	50 g/L Sodium Thiosulphate
Primary standard	0.0125237 N Potassium Iodate
Accuracy	± 0.5 µmol L^{-1}
Sample Container type	140 mL glass iodine determination flasks with glass stopper
Sample Storage	Samples stored in the hydrochemistry lab until analysis within 72 hrs.
Analyst	Kurt Debruille, Julie Janssens, Merinda McMahon, and Stephen Tibben

Dissolved Oxygen Method

Scripps Institution of Oceanography (SIO) method is used for dissolved oxygen analysis. The method is based on the whole bottle modified Winkler titration of Carpenter (1965) with modifications by Culberson *et al* (1991).

Method summary: The sample is collected in an iodine determination flask of known volume. To the sample, 1 mL of manganese (II) chloride solution is added, followed by 1 mL of alkaline iodide solution. The flask is then stoppered and inverted at least 30 times. Dissolved oxygen in the sample oxidizes an equivalent amount of Mn (II) to Mn (IV) which forms a precipitate. Just before titration, the sample is acidified, reducing Mn (IV) back to the divalent state and liberating an equivalent amount of iodine. The iodine is titrated with a standardised thiosulphate solution using a Metrohm

Dosimat fitted with a 1 mL burette. The titration endpoint is determined by measuring the decrease in the UV absorption at 365 nm.

The thiosulphate solution is standardised by with a 10 mL aliquot of potassium iodate primary standard. A blank correction is also determined from the difference between two titres of consecutive additions of 1 mL aliquots of potassium iodate to the same blank sample. The standardisation is conducted at least once every 24 hours, when samples are being assayed.

The output from the SIO instrument software is imported into HyPro and collated with the CTD deployment meta-data.

CTD Dissolved Oxygen vs Bottle Dissolved Oxygen

For this voyage, the difference between the unprocessed (uncorrected) CTD value and the measured bottle value is generally between 6 – 20 µmol L^{-1}. The larger differences are often observed with sudden changes around the thermocline.

The unprocessed CTD values are adjusted (corrected) by DAP using the dissolved oxygen bottle results. The corrected values are not reported in the hydrology set. Please refer to IN2026_V02 CTD data on CSIRO marlin metadata system for corrected sensor data.

Dissolved Oxygen Instrument titrant: thiosulphate normality and blank correction

The variation in thiosulphate concentration remains within the QC parameter of less than 0.0005 N between standardisations. The blank correction, which accounts for oxidisable species in the reagents and in the Milli-Q water that is added to the KIO_3 aliquot before the titration, is used in the calculation of the thiosulphate normality.

The mean normality of thiosulphate for this voyage was:

Mean: 0.0201540 N SD: 0.000079 n = 9

The mean blank concentration was:

Mean: 0.0007924 mL SD: 0.0001853 n = 9

Nutrients

Nutrient Measurement Parameters

Table 11. Nutrient measurement parameters analysed with Seal AA500 segmented flow analyser. All instrument parameters, reagent batches, and instrument events are logged for each analysis run. This information is available on request.

Details					
Instrument	Seal AA500 segmented flow analyser				
HyPro version	5.9				
Operating Software	AACE 8.06				
Hydrochemistry Sampling Method	WI_Nut_001				
Hydrochemistry analysis method	SOP001	SOP002	SOP003	SOP003	SOP004
Nutrients analysed	Silicate ($SiO4^{4-}$)	Phosphate (PO_4^{3-})	Nitrate + Nitrite (NO_x)	Nitrite (NO_2^-)	Ammonium (NH_4^+)
Top concentration (µmol L^{-1})	112.0	3.0	36.4	1.4	2.0
Method detection limit (MDL) (µmol L^{-1})	0.2	0.02	0.02	0.02	0.02
Stock standards	Made on 11th of February 2026 in 1L HDPE bottle				
Intermediate standards	Prepared every 72 hours in 30 mL polypropylene tubes. Reused after acid wash with 10% hydrochloric acid solution.				
Working standards	Prepared every 24-48 hours in 30 mL polypropylene tubes. Reused after acid wash with 10% hydrochloric acid solution.				
Reference Material	KANSO RMNS lot CO				

Sample Container	CTD samples: 50 mL HDPE with screw cap lids. Reused after acid wash with 10% hydrochloric acid solution. Underway samples: 30 mL PP tube with screw cap lids. Reused after acid wash with 10% hydrochloric acid solution.
Sample Storage	< 4 hours at room temperature after collection or < 24 hours at 4°C after collection, samples returned to room temperature prior to analysis.
Sample preparation	No filtration.
Analysts	Julie Janssens and Stephen Tibben

Nutrient Methods

Nutrient samples are analysed using a Seal AA500 segmented flow auto-analyser, equipped with 10 mm flow-cells.

Silicate (SOP001): colourimetric, molybdenum blue method. Based on Armstrong et al. (1967). Silicate in seawater is reacted with acidified ammonium molybdate to produce silicomolybdic acid. Tartaric acid is added to remove the phosphate molybdic acid interference. Tin (II) chloride is then added to reduce the silicomolybdic acid to silicomolybdous acid and its absorbance is measured at 660 nm.

Phosphate (SOP002): colourimetric, molybdenum blue method. Based on Murphy and Riley (1962) with modifications from the NIOZ-SGNOS[1] Practical Workshop 2012 optimizing the antimony catalyst/phosphate ratio and the reduction of silicate interferences by pH. Phosphate in seawater forms a phosphomolybdenum complex with acidified ammonium molybdate. It is then reduced by ascorbic acid, and its absorbance is measured at 880 nm.

Nitrate (SOP003): colourimetric, Cu-Cd reduction – naphthylenediamine method. Based on Wood et.al (1967). Nitrate is reduced to nitrite by first adding an ammonium chloride buffer then sending it through a copper - cadmium column. Sulphanilamide is added under acidic conditions to form a diazo compound. This compound is coupled with 1-N-naphthly-ethylenediamine di-hydrochloride to produce a magenta azo complex, and its absorbance is measured at 540 nm.

Nitrite (SOP003): colourimetric, naphthylenediamine method. As per nitrate method without the copper cadmium reduction column and buffer. Absorbance measured at 540 nm.

Ammonium (SOP004): fluorescence, ortho-phtaldiadehyde method. Based on Kérouel and Aminot (1997). Ammonium reacted with ortho-phtaldialdehyde and sulphite at a pH of 9.0-9.5 to produce an intensely fluorescent product. Its emission is measured at 460 nm after excitation at 370 nm.

SOP methods can be obtained from the CSIRO Oceans and Atmosphere Hydrochemistry Group.

[1] Royal Netherlands Institute for Sea Research – Study Group on Nutrient Standards.

HyPro Processing Summary for Nutrients

After a run, the raw absorbance and fluorescence data is exported from the instrument and processed by HyPro. For each analyte, HyPro re-constructs the peak traces and defines peak window, which corresponds to the plateau region used to determine the peak heights. HyPro then constructs the calibration curve and applies corrections for carry-over, baseline, and sensitive drifts, then the nutrient concentrations for each sample are calculated. The corrections are quantified using dedicated solutions included in every run.

HyPro applies specific criteria to identify suspect calibration points, noisy peaks, method detection limits above the nominal threshold, and duplicate sample results that do not match.

Suspect calibration points are given less weight when fitting the calibration curve. The cut-off limits for acceptable calibration data are as followed:

- ±0.5% of the concentration of the top standard for silicate and nitrate+nitrite (as per WOCE[1]).
- 0.02 µmol L^{-1} for phosphate, nitrite, and ammonium.

HyPro classifies data quality as good, suspect, or bad and flags the results accordingly. The Flag key can be found in Appendix, Data Quality Flag Key. Missing or suspect nutrient data is listed in Appendix, Missing or Suspect Nutrient Data.

[1] World Ocean Circulation Experiment

Table 12. HyPro Processing Parameters. All instrument parameters and reagent batches and operation events are logged for each analysis run. This information is available on request.

Result Details	Silicate	Phosphate	Nitrate + Nitrite	Nitrite	Ammonium
Data Reported as	µmol L^{-1}	µmol L^{-1}	µmol L^{-1}	µmol L^{-1}	µmol L^{-1}
Calibration Curve fit	Linear	Linear	Quadratic	Quadratic	Linear

# of points in Calibration	6	6	6	6	6
Forced through zero	N	N	N	N	N
Matrix correction	N	N	N	N	N
Blank correction	N	N	N	N	N
Refractive Index Blank (RIB) correction	Y	Y	Y	Y	N
Peak window defined by	HyPro	HyPro	HyPro	HyPro	HyPro
Carryover correction	Y	Y	Y	Y	Y
Baseline drift correction	Y	Y	Y	Y	Y
Sensitivity drift correction	Y	Y	Y	Y	Y
Data Adjusted for RMNS variance	N	N	N	N	N
Medium of Standards	Low nutrient seawater (LNSW) collected in June 2024. Sub-lot passed through a 5-micron filter (filtered in February 2026) and stored in 20 L carboys in the hydrochemistry laboratory at 20°C.				
Medium of Baseline	18.2 MΩ water. Dispensed from the Milli-Q IQ 7010 system.				
Duplicate samples	CTD: Niskin fired at the greatest depth for each CTD deployment were analysed in duplicate. Single samples were analysed for remaining depths.				
Note	The reported data is not corrected to the RMNS. Per deployment RMNS data is provided in supporting document.				

Refractive Index Blank (RIB) measurement and correction

The refractive index blank (RIB) is an optical interference caused by the difference in refraction between seawater and Milli-Q water. This effect alters light transmission and scattering within the flow cell, resulting in baseline shifts and potential underestimation or overestimation in absorbance measurements during colorimetric analysis (Kirkwood, D.S., 1996).

To quantify RIB, the non-coloured reagent method was employed. In this approach, Milli-Q water and LNSW were analysed using the complete reagent set described in the Nutrients Method section above, except for the colour-generating chemicals. Specifically, 1-N-naphthyl-ethylenediamine dihydrochloride was omitted for NOx and NO2, while ammonium molybdate was excluded for silicate and phosphate. No RIB effect was observed for ammonium channel.

At the end of an analysis run, the full suite of reagents was switched to the non-coloured reagent setup, and the percentage difference between Milli-Q water and LNSW was recorded for each channel using AACE software. This percentage was then converted into concentration values using a proportional ratio calculation, where the highest calibrant nominal concentration and its corresponding peak height percentage were used as reference points.

The average RIB values from multiple nutrient analysis runs overtime are presented in Table 13. RIB value was entered into HyPro where nutrient data was corrected.

Table 13. Average refractive index blank (RIB) offset value for each channel used for correction on this voyage (Units: µmol L^{-1}, n = 14).

Silicate	Phosphate	Nitrite	Nitrate + Nitrite
0.0429 ± 0.0842	0.0290 ± 0.0056	0.0159 ± 0.0051	0.0206 ± 0.0239

Accuracy - Reference Material for Nutrient in Seawater (RMNS)

Descriptive statistics are used to ascertain the accuracy and precision of the analysis from the repetitive measurement of the RMNS for silicate, phosphate, NOx, nitrite and ammonium in seawater.

For this voyage, Japanese KANSO certified RMNS lot CO was assayed in triplicates in each run to monitor accuracy (Table 14). RMNS CU and CW were only analysed in the characterisation (run nut001) run as additional accuracy monitoring at the start of the voyage without samples. An internal bulk quality control (BQC) was also analysed in each analysis run.

The GO-SHIP criteria (Hyde *et al*., 2010), Appendix, GO-SHIP Specifications, specifies using 1-3% of full scale (depending on the nutrient) as acceptable limits of accuracy.

KANSO publishes the RMNS nutrient values in µmol kg^{-1}. These are converted to µmol L^{-1} at 21°C. NO_x is derived by summing the NO_3^- and NO_2^- values.

Table 14. RMNS certified concentrations ± expanded uncertainty (U) at 21°C. Units: µmol L^{-1}

RMNS	Silicate	Phosphate	Nitrite	Nitrate + Nitrite	Ammonium
Lot CO	35.5515 ± 0.1638	1.2052 ± 0.0143	0.0410 ± 0.0410	16.2808 ± 0.1946	N/A

Table 15. RMNS CO statistics for of this voyage. Units: µmol L^{-1}

RMNS CO	Silicate	Phosphate	Nitrite	Nitrate + Nitrite	Ammonium
Mean	35.789	1.214	0.050	16.399	N/A
Standard deviation	0.149	0.007	0.005	0.066	N/A

RMNS plots

The measured RMNS values for each nutrient analysis run on this voyage is shown in plots below. The green, pink, and red contour lines represent 1%, 2% and 3% or 1*MDL, 2*MDL and 3*MDL (MDL = 0.02 µmol L^{-1}) deviation from the RMNS certified mean value. The blue line is the manufacturer's expanded uncertainty of the certified value. The measured RMNS values per CTD deployments are provided in supporting document available on CSIRO data trawler.

For this voyage, results for RMNS lot CO show high agreement with certified values, with calculated results falling within the expanded uncertainty. The plot of RMNS lot CO analysed in each channel are shown in figure 3 to figure 6.

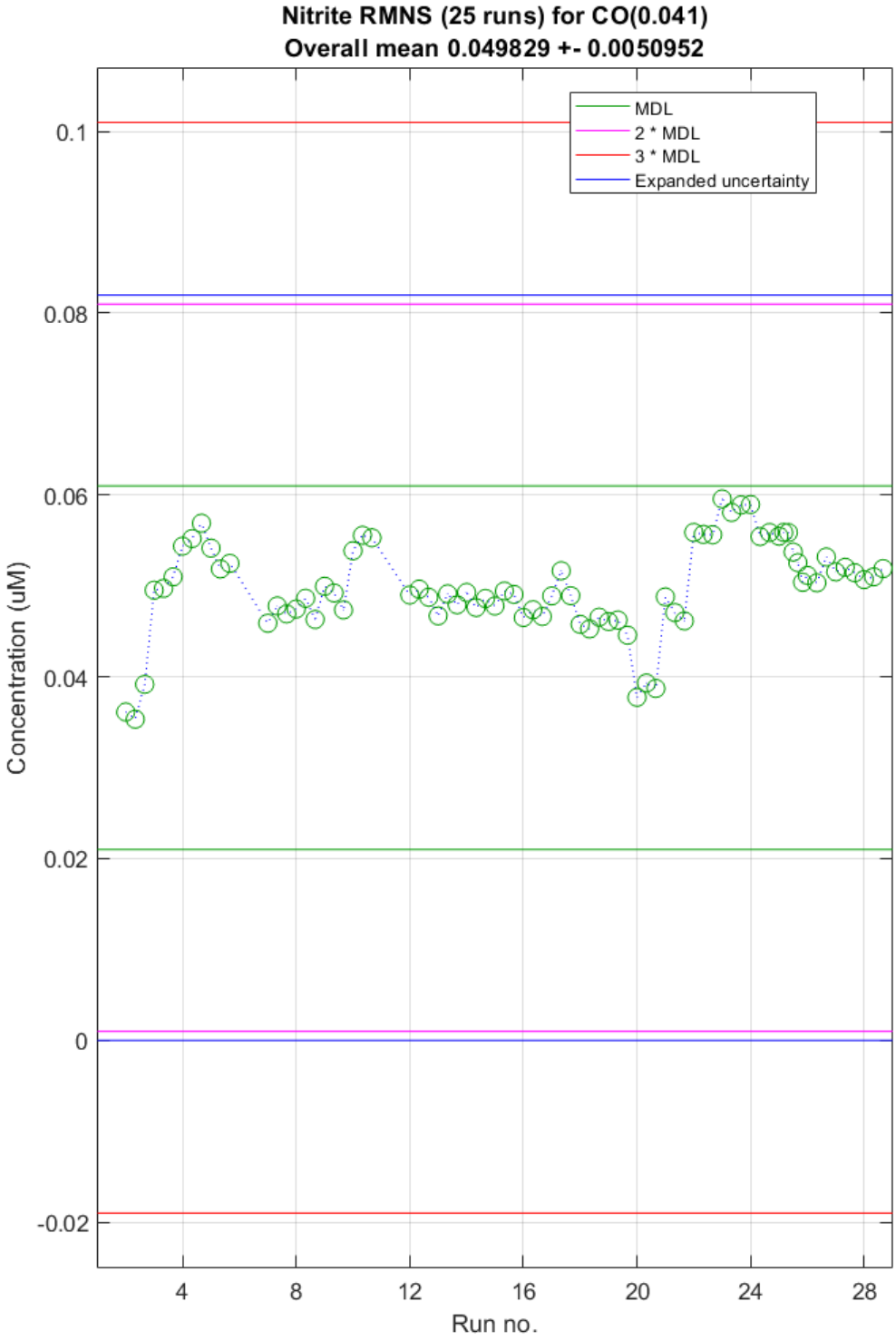

Figure 3. Nitrite RMNS lot CO plot. Units: µmol L^{-1}.

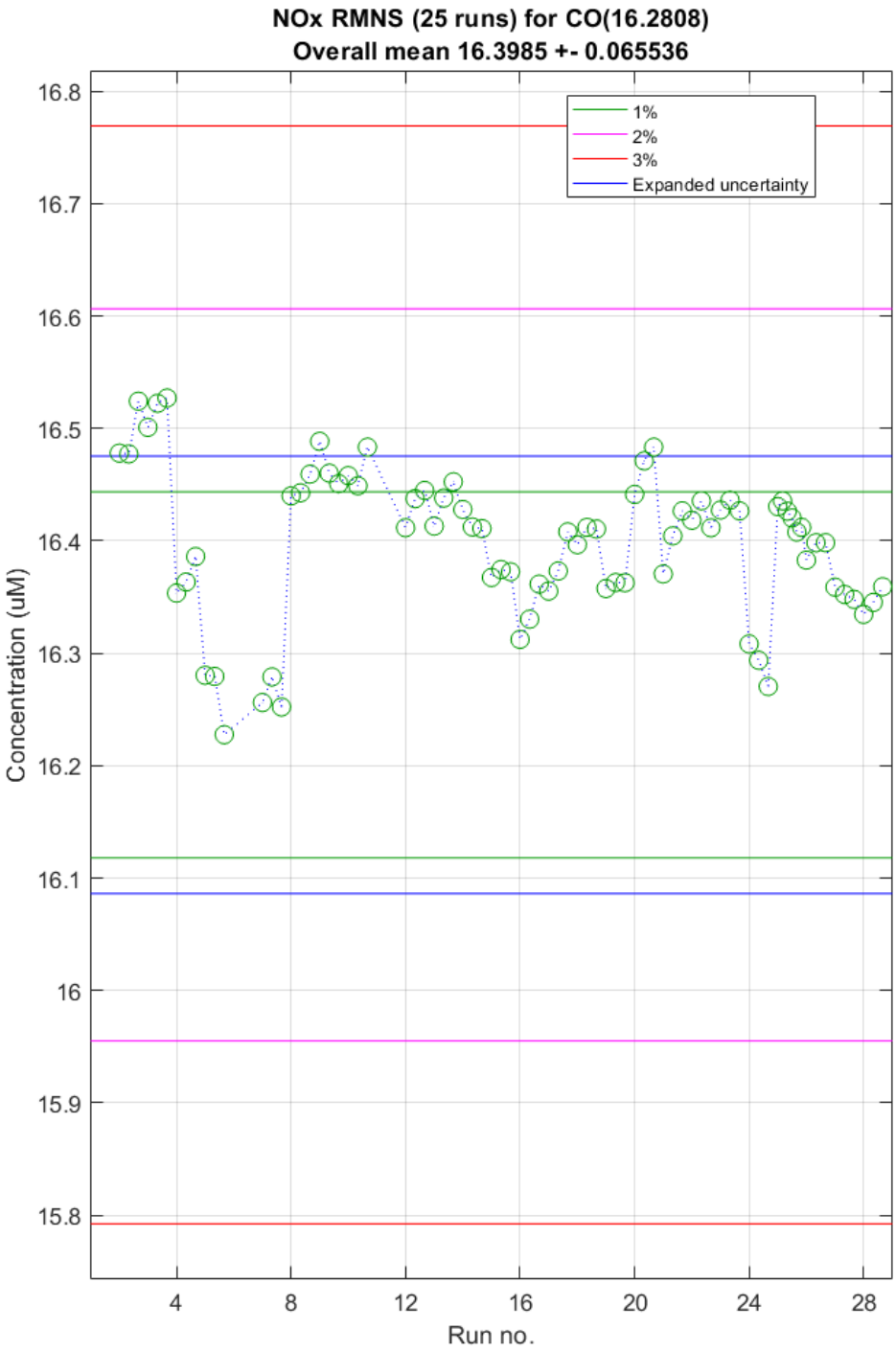

Figure 4. Nitrate + Nitrite (NOx) RMNS lot CO plot. Units: µmol L^{-1}.

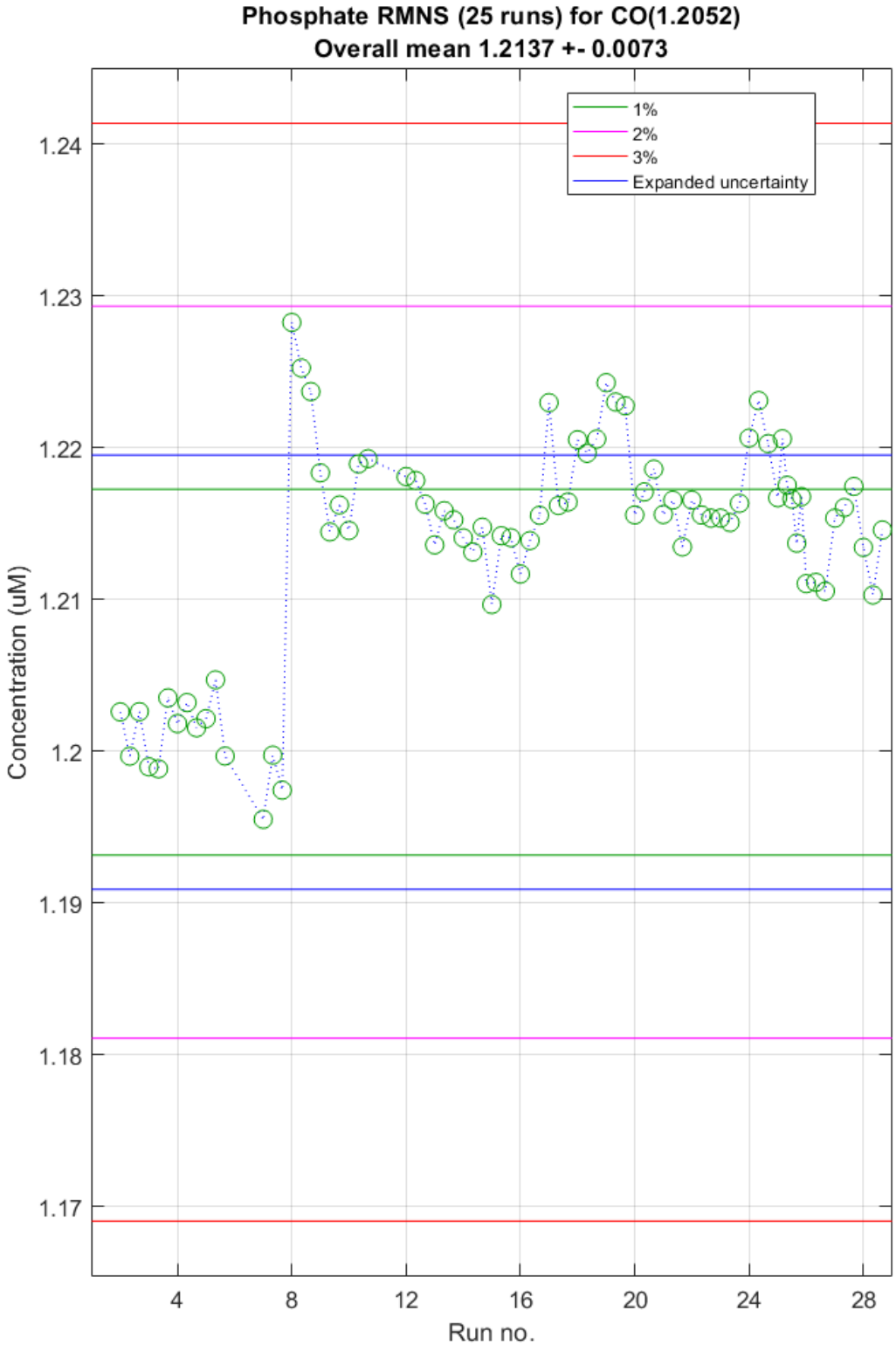

Figure 5. Phosphate RMNS lot CO plot. Units: Units: µmol L^{-1}.

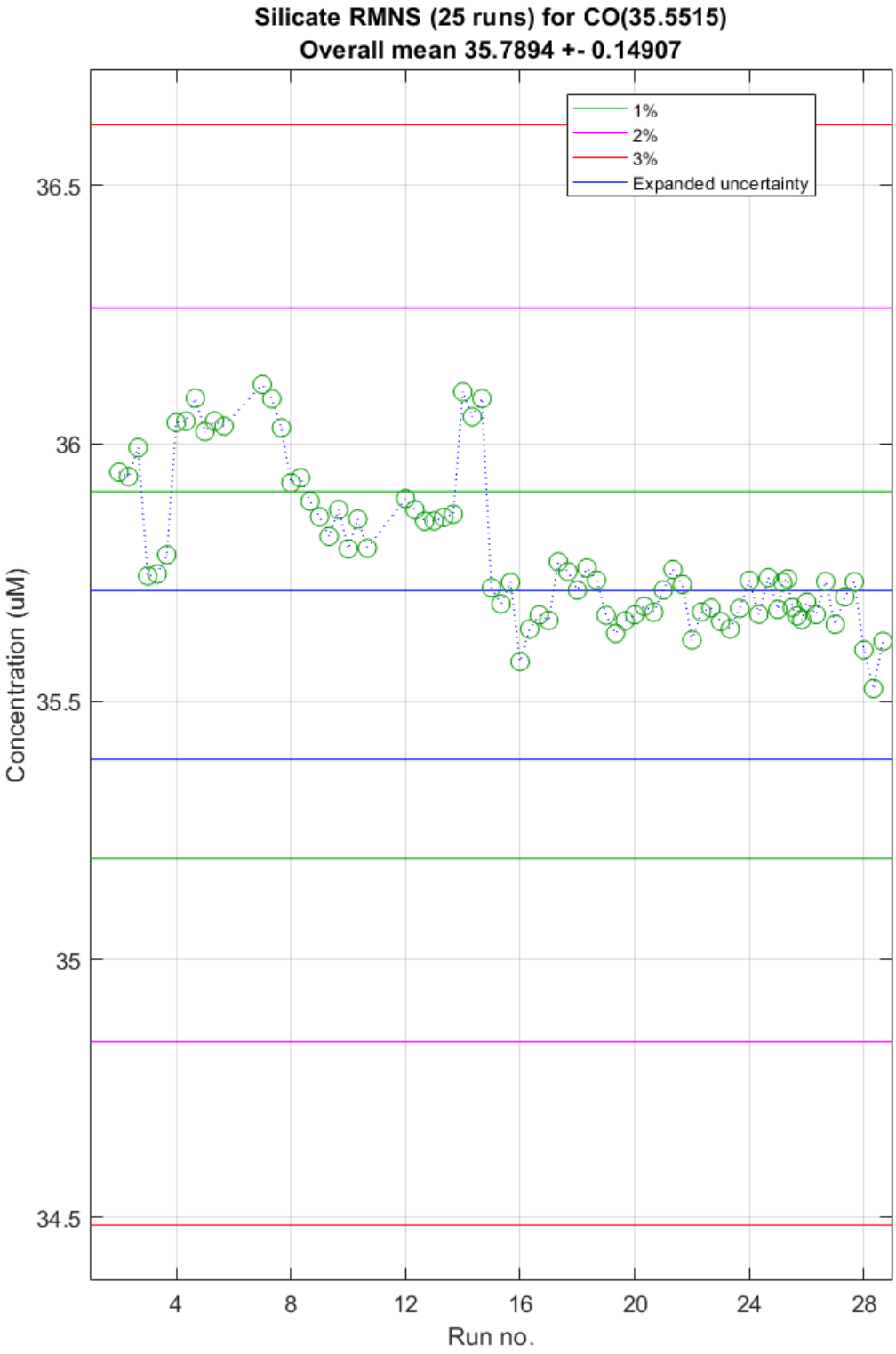

Figure 6. Silicate RMNS lot CO plot. Units: Units: µmol L^{-1}.

Measurement Uncertainty

The CSIRO hydrochemistry method measurement uncertainty (MU) has been calculated for each nutrient based on the variation in the calibration curve, calibration standards, pipette and glassware calibration, and precision of the RMNS over time (Armishaw 2003).

Table 16. CSIRO Hydrochemistry nutrient analysis uncertainty values. Units: µmol L^{-1}

Calculated Measurement Uncertainty at 1 µmol L^{-1}				
Silicate	**Phosphate**	**Nitrite**	**Nitrate + Nitrite**	**Ammonium**
±0.017	±0.024	±0.140	±0.019	±0.30

The reported uncertainty is an expanded uncertainty using a coverage factor of 2 giving a 95% level of confidence.

Method Detection Limit for Nutrients

The method detection limit (MDL) is defined as three times the standard deviation (SD) of the LNSW results (National Association of Testing Authorities 2013). The MDL is used to assess the precision of the analysis at low nutrient concentrations.

Table 17. AA500 auto analyser MDL statistics for this voyage. The mean and standard deviation are calculated from every analytical run performed over the voyage. Units: µmol L^{-1}.

MDL	**Silicate**	**Phosphate**	**Nitrite**	**Nitrate + Nitrite**	**Ammonium**
Nominal MDL	**0.2**	**0.02**	**0.02**	**0.02**	**0.02**
Mean	0.02	0.005	0.003	0.006	0.002
Standard deviation	0.01	0.002	0.002	0.003	0.001

Sampling Precision

Sampling precision is typically determined using the CTD test deployment (CTD 001) where multiple bottles are fired the same depth, each of which is then sampled as replicates for hydrochemistry nutrient analysis. The mean and standard deviation of nutrients analysed on test deployment is shown in table 18.

Duplicate nutrient samples are also collected from the greatest depth of subsequent CTD deployments. For nutrients analysis, the sampling precision is considered good if the difference from the mean of duplicate measurements is less than the nominal method detection limit (Table 17). The exception is for NO_x (nitrate + nitrite), which uses the limit of 0.06 µmol L^{-1}. Duplicate samples that exceed the limit are flagged. These are tabulated in Appendix, Data Quality Flag Key.

Table 18. Test cast deployment at 1035 dbar. Bottle rosette position (RP) 1-36. Units: µmol L^{-1}.

Replicates	Silicate	Phosphate	Nitrite	Nitrate + Nitrite	Ammonium
Mean	61.48	2.43	0.00	35.30	0.00
Standard deviation	0.10	0.01	0.00	0.04	0.00

Temperature

Hydrochemistry lab and nutrient analyser

Ambient conditions in the hydrochemistry laboratory and on the segmented flow analyser were monitored at the following locations:

- Hydrochemistry lab temperature: positioned in close proximity to the autoanalyser
- Nutrient sample pump temperature: positioned on the pump tubes where nutrient samples and reagents are introduced into the analyser

Temperature data was measured using Ruuvi temperature logger and monitored in Grafana. A time series plot of hydrochemistry laboratory temperature plot throughout the voyage is shown below. A complete log of temperature is available upon request through CSIRO data centre. The average analyser pump temperature of the analyser during each nutrients analysis is provided in supporting documents available on CSIRO data trawler.

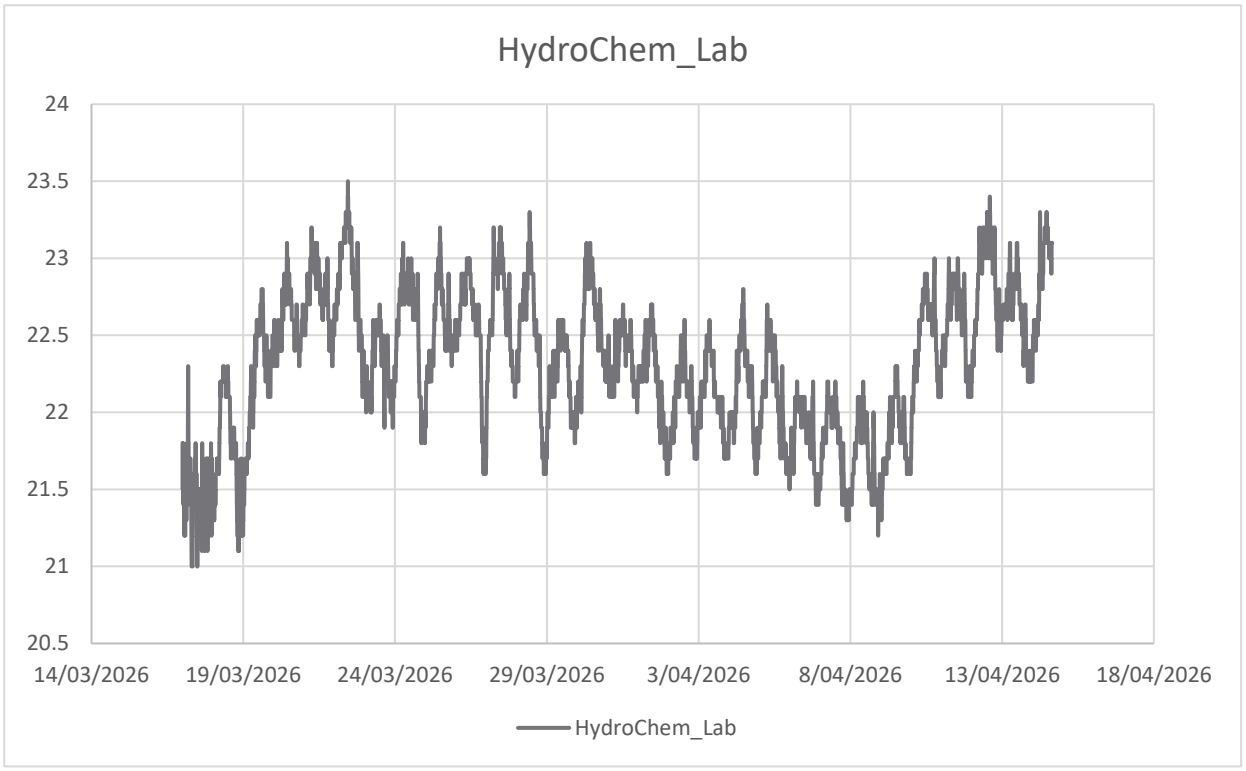

Figure 8. Hydrochemistry lab Ruuvi sensor; scale is 20.5 to 24.0, mean: 22.3.0°C, SD: 0.5°C.

Salinity laboratory

Ambient conditions in the salinity laboratory were monitored using a Ruuvi temperature logger positioned near the area where sample crates were stored. Temperature data was recorded and visualised in Grafana. A time series plot of salinity lab temperature throughout the voyage is shown below. A complete log of temperature is available upon request through CSIRO data centre.

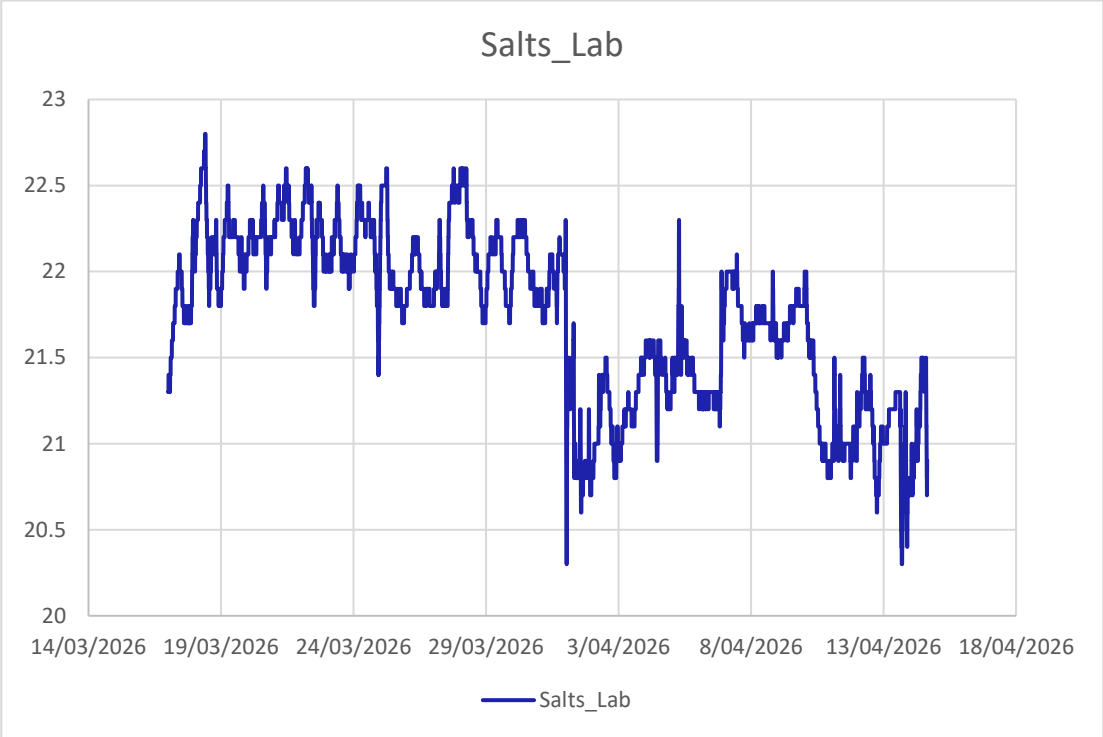

Figure 9. Hydrochemistry lab Ruuvi sensor; scale is 20.0°C to 23.0°C, mean: 21.7°C, SD: 0.5°C.

Appendix

Salinity: Reference material used

OSIL IAPSO Standard Seawater	
Batch	P168
Use by date	1 December 2026
K_{15}	0.99993
PSU	34.997

Nutrients: RMNS correction

The submitted nutrient results do NOT have RMNS corrections applied. The measured RMNS value per CTD deployment is provided in supporting document available on CSIRO data trawler.

How to use the RMNS for correction

Ratio = Certified RMNS Concentration/Measured RMNS Concentration in each run

Corrected Concentration = Ratio x Measured Nutrient Concentration

How to use the RMNS for smoothing

Ratio = Average RMNS Concentration across voyage/Measured RMNS Concentration in each run

Corrected Concentration = Ratio x Measured Nutrient Concentration

Missing or Suspect Salinity Data

Data is flagged based on CTD sampling log notes, observations during analysis, and examination of depth profile plots (Appendix, Data Quality Flag Key).

CTD	RP	Flag	Reason for Flag
51	07	141	Broken bottle

Missing or Suspect Dissolved Oxygen Data

Data is flagged based on CTD sampling log notes, observations during analysis, and examination of depth profile plots (Appendix, Data Quality Flag Key).

CTD	RP	Flag	Reason for Flag
NA	NA	NA	

Missing or Suspect Nutrient Data

Data is flagged based on CTD sampling log notes, observations during analysis, and examination of depth profile plots (Appendix, Data Quality Flag Key).

Note: Within the .csv file many ammonium samples are flagged 63 – below nominal detection limit. Ammonium only occurs in the upper few hundred metres of the ocean and within the Chlorophyll maximum, effectively its concentration is zero at all other depths. Due to the difficulty in analysing ammonium in seawater often the zero concentrations will be reported as a negative value, this is due to the baseline Milli-Q water becoming slightly contaminated due to the air quality within the laboratory, meaning the baseline is slightly greater than zero concentration. These ammonium samples are not reported in this table.

CTD	RP	Analyte	Flag	Reason for Flag
13	01	NH_4^+	133	Data is bad, marked by operator. Apparent contamination since duplicate is outside of set limits.
27	01	NH_4^+	133	Data is bad, marked by operator. Apparent contamination since duplicate is outside of set limits.

Data Quality Flag Key

Flag	Description	
0	Data is GOOD	
63	Nutrients only.	Data below nominal detection limit.

65	Data is SUSPECT.	Nutrients only: Absorbance peak shape, measured by the instrument, is marginally outside set limits.
69	Data is SUSPECT.	Duplicate data is outside of set limits (software). Data point is an outlier on the depth profile plot (operator). Tagged by software or operator
79	Data is SUSPECT.	Nutrients only. Measured Method Detection Limit (MDL) for the analysis run is greater than the nominal MDL. All samples in that run tagged.
129	Data is BAD.	Nutrients Only. Absorbance peak exceeds the maximum value that can be measured by the instrument.
133	Data is BAD.	Set by operator.
134	Data is BAD.	Nutrients Only. Absorbance peak shape of calibrant, measured by the instrument, is outside of set limits (software).
141	NO Data.	Used in netcdf results file. Not used in csv results file.

GO-SHIP Specifications

Salinity

Accuracy of 0.001 is possible with Autosal™ salinometers and concomitant attention to methodology. Accuracy with respect to one particular batch of standard Seawater can be achieved at better than 0.001 PSS-78. A precision of approximately 0.0002 PSS-78 is possible following the methods of Kawano with great care and experience. Air temperature stability of ± 1°C is very important and should be recorded [2].

Dissolved Oxygen

Target accuracy is that 2 sigma (standard deviation) should be less than 0.5% of the highest concentration found in the ocean. Precision or reproducibility (2 sigma) is 0.08% of the highest concentration found in the ocean.

$Si(OH)_4$

Approximately 1-3% accuracy[1], 0.2% precision[3], full scale.

PO_4^{3-}

Approximately 1-2% accuracy[1], 0.4% precision[3], full scale.

NO_3^-

Approximately 1% accuracy[1], 0.2% precision[3], full scale.

Notes

[1] If no absolute standards are available then accuracy should be taken to mean the reproducibility presently obtainable in the better laboratories.

[2] Keeping constant temperature in the room where salinities are determined greatly increases their quality. Also, room temperature during the salinity measurement should be noted for later interpretation if queries occur. Additionally, monitoring and recording the bath temperature is also recommended. The frequent use of IAPSO Standard Seawater is endorsed. To avoid the changes that occur in Standard Seawater, the use of the most recent batch is recommended. The bottles should also be used in an interleaving fashion as a consistency check within a batch and between batches.

[3] Developments of reference materials for nutrients are underway that will enable improvements in the relative accuracy of measurements and clearer definition of the performance of laboratories when used appropriately and the results are reported with the appropriate meta-data.

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