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# **GO-SHIP A16N 2023 Leg 2: NOAA Quality Control and Data Analysis Report for the Inorganic Carbon Parameters**

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Miami, Florida

August 2025

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# **GO-SHIP A16N 2023 Leg 2: NOAA Quality Control and Data Analysis Report for the Inorganic Carbon Parameters**

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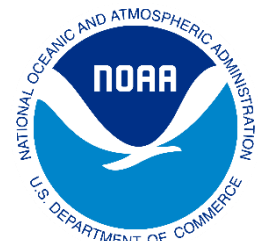
August 2025

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## Acronyms

|                    |   |
|--------------------|---|
| GO-SHIP            | Global Ocean Ship-Based Hydrographic Investigations Program |
| AOML               | Atlantic Oceanographic and Meteorological Laboratory        |
| CIMAS              | Cooperative Institute for Marine and Atmospheric Studies    |
| GOMO               | Global Ocean Monitoring and Observing Program               |
| NSF                | National Science Foundation                                 |
| QC                 | Quality control   |
| CRM                | Certified reference material                                |
| CO <sub>2</sub>    | Carbon dioxide  |
| DIC                | Total dissolved inorganic carbon                            |
| TA                 | Total alkalinity  |
| $f\text{CO}_2$     | Fugacity of carbon dioxide                                  |
| WOCE               | World Ocean Circulation Experiment                          |
| CTD                | Conductivity/temperature/depth                              |
| CCHDO              | Clivar and Carbon Hydrographic Data Office                  |
| PI                 | Principal investigator                                      |
| RSMAES             | Rosenstiel School of Marine, Atmospheric, and Earth Science |
| PMEL               | Pacific Marine Environmental Laboratory                     |
| mCP                | meta-cresol purple  |
| $K_1, K_2$         | Carbonic acid dissociation constants                        |
| $K_{\text{HSO}_4}$ | Bisulfate dissociation constant                             |
| $K_{\text{HF}}$    | Hydrogen fluoride dissociation constant                     |
| $B_{\text{T}}/S$   | Total boron to salinity ratio                               |
| $S_{\text{P}}$     | Salinity, practical scale                                   |
| O <sub>2</sub>     | Oxygen  |
| Stdev              | Standard deviation  |

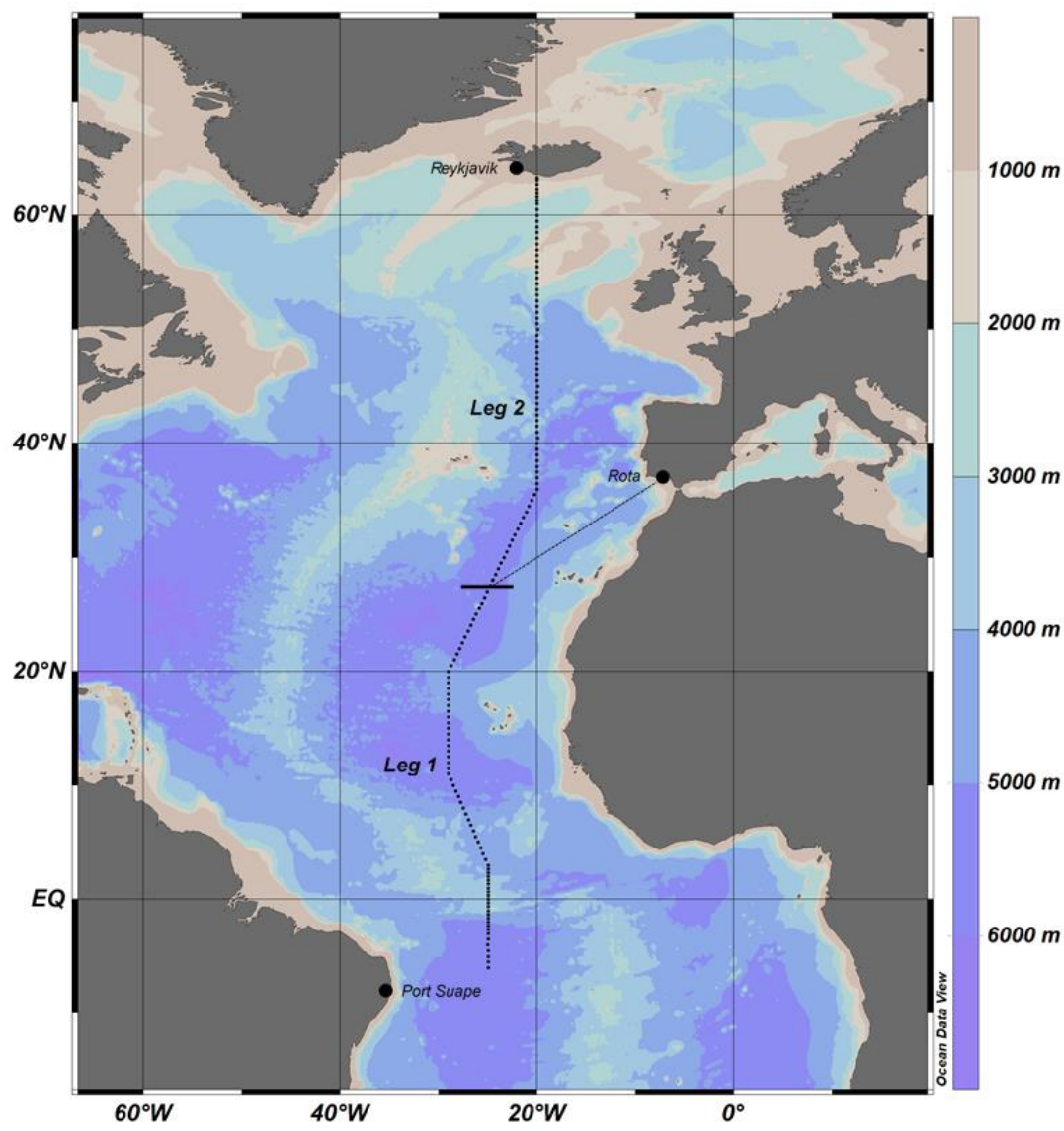
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## Abstract

The Global Ocean Ship-Based Hydrographic Investigations Program (GO-SHIP) A16N Leg 2 2023 cruise took place onboard the *NOAA Ship Ronald H. Brown* from April 13 to May 9, 2023, traveling between Rota, Spain and Reykjavik, Iceland. This technical report documents and details the quality control (QC) procedures and data analyses of the inorganic carbon parameter measurements (total alkalinity, TA ( $\mu\text{mol kg}^{-1}$ ); total dissolved inorganic carbon, DIC ( $\mu\text{mol kg}^{-1}$ ); pH on the total scale at 25 °C,  $\text{pH}_\text{T}(25)$ ; and fugacity of  $\text{CO}_2$  at 20 °C,  $f\text{CO}_2(20)$  ( $\mu\text{atm}$ )) from 75 conductivity/temperature/depth (CTD) stations. After preliminary QC analyses at sea, secondary QC analyses and internal consistency assessments were conducted in this report as a means to standardize the QC protocols and ensure a fully consistent data set for all four inorganic carbon parameters. Analyses highlight that the inorganic carbon measurements for the A16N Leg 2 2023 cruise follow best-practice measurement protocols.

## 1. Introduction

The U.S. Global Ocean Ship-based Hydrographic Investigations Program ([GO-SHIP](#)) A16N 2023 Leg 2 cruise, led by Chief Scientist Leticia Barbero and Co-Chief Scientist Laura Cimoli, took place onboard the *NOAA Ship Ronald H. Brown* from April 13 to May 9, 2023, traveling between Rota, Spain and Reykjavik, Iceland (Fig. 1). Conductivity/temperature/depth (CTD) casts were conducted at 75 stations, and included measurements of physical properties (salinity (via conductivity), temperature, depth (via pressure)), inorganic carbon parameters (total alkalinity, TA; total dissolved inorganic carbon, DIC; pH on the total scale at 25 °C, pH<sub>T</sub>(25); fugacity of carbon dioxide (CO<sub>2</sub>) at 20 °C, *f*CO<sub>2</sub>(20)), nutrient concentrations (nitrate, nitrite, phosphate, silicate), dissolved oxygen concentration, trace gases (chlorofluorocarbons, CFCs; sulfur hexafluoride, SF<sub>6</sub>; nitrous oxide, N<sub>2</sub>O), and other ancillary measurements including biological sampling and organic concentrations (dissolved organic carbon). The full cruise report and complete dataset are available for download on the Clivar and Carbon Hydrographic Data Office (CCHDO) website (EXPCODE: 33RO20230413; <https://cchdo.ucsd.edu/cruise/33RO20230413>). This report documents and details the quality control (QC) procedures and data analyses of the inorganic carbon parameter measurements (TA (μmol kg<sup>-1</sup>), DIC (μmol kg<sup>-1</sup>), pH<sub>T</sub>(25), and *f*CO<sub>2</sub>(20) (μatm)). An analogous report contains the published information for the GO-SHIP A16N 2023 Leg 1 cruise (Schockman, 2025).



**Fig. 1.** GO-SHIP A16N 2023 Leg 1 and Leg 2 cruise tracks. The black horizontal bar denotes the cutoff between the two legs of the cruise.

## 2. Methods

### 2.1 Data Collation and Primary QC

Details of the measurement protocols for all parameters can be found in the full cruise report. The principal investigators (PI) and analysts for the four inorganic carbon parameters are

given in Table 1, with a full list of PIs and analysts for all cruise measurements in the full cruise report. Every sample on the cruise was assigned a sample ID: sample ID = 10000\*station + 100\*cast + bottle number. Note that the A16N 2023 Leg 2 stations are numbered 76–150 to allow for cohesiveness with the A16N 2023 Leg 1 stations numbered 1–75. While onboard, initial quality flags were assigned to each inorganic carbon measurement following the World Ocean Circulation Experiment (WOCE) protocols as defined in Table 2 (WHP, 1998).

**Table 1**

PIs and analysts, along with their affiliated institutions, for each of the inorganic carbon parameter measurements. Note: RSMAES – Rosenstiel School of Marine, Atmospheric, and Earth Science; PMEL – Pacific Marine Environmental Laboratory; AOML – Atlantic Oceanographic and Meteorological Laboratory; and CIMAS – Cooperative Institute for Marine and Atmospheric Studies.

| Parameter             | PI(s)                                   | Institution            | Analyst                              | Institution   |
|-----------------------|---|------------------------|--------------------------------------|---|
| TA                    | Dr. Chris Langdon                       | U. Miami<br>(RSMAES)   | Dr. Bo Yang<br>Jessica Leonard       | U. Miami (RSMAES)<br>U. Miami (RSMAES)                    |
| DIC                   | Dr. Richard Feely<br>Dr. Rik Wanninkhof | NOAA PMEL<br>NOAA AOML | Charles Featherstone<br>Dana Greeley | NOAA AOML<br>NOAA PMEL                                    |
| pH <sub>T</sub> (25)  | Dr. Chris Langdon                       | U. Miami<br>(RSMAES)   | Laura Stieghorst<br>Seamus Jameson   | U. Miami (RSMAES)<br>U. Miami (RSMAES)/<br>San Jose State |
| fCO <sub>2</sub> (20) | Dr. Rik Wanninkhof                      | NOAA AOML              | Patrick Mears<br>Dr. Leah Chomiak    | U. Miami (CIMAS)<br>U. Miami (CIMAS)                      |

**Table 2**

WOCE data quality flags used in the GO-SHIP A16N 2023 Leg 2 dataset for the inorganic carbon water samples (WHP, 1998).

| Flag Value | Definition   |
|------------|--|
| 2          | Acceptable measurement                                 |
| 3          | Questionable measurement                               |
| 4          | Bad measurement  |
| 6          | Mean of replicate measurements                         |
| 9          | Sample not drawn for this measurement from this bottle |

During and after the cruise, some adjustments were made to the inorganic carbon measurements unique to each parameter. For DIC, two systems (AOML3 and AOML4) were concurrently used throughout the cruise. A pipette used in the AOML3 system broke during shipping prior to the cruise, requiring that the volume of the new replacement pipette be recalibrated after the cruise. This resulted in a small, post-cruise adjustment to samples measured on that system. The average absolute difference between the AOML3 initial DIC values and corrected DIC values after the post-cruise pipette calibration was  $0.39 \pm 0.18 \mu\text{mol kg}^{-1}$ . The corrected DIC values for AOML3 are the values provided in the CCHDO dataset. For  $\text{pH}_T$ , measurements were performed near  $25^\circ\text{C}$ , with the exact temperature recorded, and then adjusted to a temperature of  $25^\circ\text{C}$  for reporting purposes (denoted as  $\text{pH}_T(25)$ ). Additionally,  $\text{pH}_T$  measurements were corrected onboard for small perturbations caused by the indicator dye (meta-cresol purple, mCP) on the sample (for more details, see the full cruise report). A16N 2023 Leg 1 and Leg 2 used separate batches of mCP. For  $f\text{CO}_2$ , measurements were performed near  $20^\circ\text{C}$ , with the exact temperature recorded, and then adjusted to a temperature of  $20^\circ\text{C}$  for reporting purposes (denoted as  $f\text{CO}_2(20)$ ). Additionally,  $f\text{CO}_2$  samples were calibrated using standard gases measured before and after each set of up to 12 samples (for more details, see the full cruise report).

During A16N 2023 Leg 1, the recorded instrument standard deviations were observed to be high for all  $f\text{CO}_2$  measurements. To remedy this, the gas analyzer (LI-COR) was replaced between Leg 1 and Leg 2. Subsequent QC checks were performed by the parameter leads after all corrections and adjustments were made to flag any noticeable outliers.

The precision of measurements for each of the inorganic carbon parameters was assessed through routine duplicate measurements on a subset of samples throughout the cruise (Tables 3–6; see Additional Tables section below). For full, 24-bottle Niskin casts, TA and  $\text{pH}_\text{T}(25)$  generally selected two sets of duplicates randomly throughout the cast. Each duplicate pair was run back-to-back during analysis. TA and  $\text{pH}_\text{T}(25)$  used one sample bottle for both measurements, so the duplicate pairs were generally the same for both parameters. For DIC, typically three sets of duplicates were randomly selected from near the bottom, mid-depth, and surface Niskin bottles. Each duplicate pair was spread out throughout the titration cell run, with duplicate measurements specifically not run back-to-back. For  $f\text{CO}_2(20)$ , generally one set of duplicates was randomly selected throughout the cast. The duplicate pair was run back-to-back during analysis. To read more details about duplicate measurements, please see the full cruise report.

## 2.2 Secondary QC

After the primary QC discussed above, the inorganic carbon data were collated to perform secondary QC checks. Measurements of TA, DIC,  $\text{pH}_\text{T}(25)$ , and  $f\text{CO}_2(20)$  with WOCE quality flags of 2, 3, 4, and 6 (Table 2) were kept for this analysis. Internal consistency of these measurements was assessed by comparing measured and calculated values for each of the inorganic carbon parameters. Generally, the closer measured and calculated values are to one another, the more internally consistent the dataset is said to be. Calculations of the inorganic carbon



parameters were made using CO2SYS (Pierrot et al., 2006; Van Heuven et al., 2011) version 3.1.1 for MATLAB (Sharp et al., 2020). All calculations were performed on the total  $\text{pH}_T$  scale using the following parameters: carbonic acid dissociation constants ( $K_1$  and  $K_2$ ) of Lueker et al. (2000), bisulfate dissociation constant ( $K_{\text{HSO}_4}$ ) of Dickson (1990), hydrogen fluoride dissociation constant ( $K_{\text{HF}}$ ) of Perez and Fraga (1987), and total boron to salinity ratio ( $B_T/S$ ) of Lee et al. (2010). Calculations generally utilized the salinities (practical scale;  $S_P$ ) from discrete bottles measured onboard unless the measured salinity value was not flagged as 2 or 6, in which case the salinity value from the CTD sensor was used.

Calculated values of a parameter  $X$  obtained using inputs of  $Y$  and  $Z$  are denoted throughout the document as ' $X(Y,Z)$ '. The difference between measured  $X$  and  $X(Y,Z)$  is a residual of  $X$  and is denoted as ' $\Delta X$ ' (i.e.,  $\Delta X = X - X(Y,Z)$ ). As all four inorganic carbon parameters were measured, and only two parameters are required for a single calculation, each inorganic carbon parameter was generally calculated using three sets of combination pairs (i.e., TA can be calculated using (DIC,  $\text{pH}_T(25)$ ), (DIC,  $f\text{CO}_2(20)$ ), and ( $\text{pH}_T(25)$ ,  $f\text{CO}_2(20)$ )). If any of the inorganic carbon parameter measurements were missing for that sample, only the available combination pairs were used. Calculations using the ( $\text{pH}_T(25)$ ,  $f\text{CO}_2(20)$ ) input pair were used for analyses in some situations, especially where one of the other inorganic carbon parameters was missing, but are generally not shown throughout the document as they are not recommended according to best practices (Patsavas et al., 2015). The residuals for each of the inorganic carbon parameters were analyzed to check for outlier sample values via a quantitative process described below.

For all 75 stations, depth profiles were created for measurements of discrete oxygen ( $\text{O}_2$ ), CTD sensor  $\text{O}_2$ , discrete  $S_P$ , CTD sensor  $S_P$ , TA, DIC,  $\text{pH}_T(25)$ , and  $f\text{CO}_2(20)$ . These depth profiles

were used in this work for visual indication of potential outliers and/or Niskin bottles fired/closed at incorrect depths.

### *2.3 Certified Reference Material (CRM) Checks Throughout the Cruise*

CRMs provided by Dr. Andrew Dickson's laboratory at Scripps Institution of Oceanography were used to assess the accuracy of both TA and DIC measurements throughout the cruise. For TA measurements, CRMs were used to standardize the HCl acid concentration used in the TA titrations and to check that the system was functioning properly. For each DIC system, CRMs were run at the beginning of a subset of sample measurements corresponding to a specific titration cell, which typically was used for one station's worth of samples. The difference between the measured CRM DIC value and certified CRM DIC value was used to adjust the system for that specific subset of measurements. For more details, see the full cruise report.

## **3. Results**

### *3.1 Primary and Secondary QC Checks*

The duplicate measurements of TA, DIC,  $\text{pH}_T(25)$ , and  $f\text{CO}_2(20)$  are provided in Tables 3–6, including both individual duplicate values and the absolute difference between the two measurements. The average  $\pm$  standard deviation (stdev;  $1\sigma$ ) of the absolute differences between duplicates for each parameter is as follows — TA:  $1.0 \pm 0.8 \mu\text{mol kg}^{-1}$  ( $n = 124$  duplicate measurement pairs); DIC:  $1.8 \pm 1.4 \mu\text{mol kg}^{-1}$  ( $n = 168$  duplicate measurement pairs);  $\text{pH}_T(25)$ :  $0.0013 \pm 0.0013$  ( $n = 145$  duplicate measurement pairs); and  $f\text{CO}_2(20)$ :  $0.5 \pm 0.3 \mu\text{atm}$  ( $0.07 \pm 0.06\%$ ) ( $n = 75$  duplicate measurement pairs) (Table 7).

**Table 7**

Inorganic carbon parameter statistics from the primary and secondary QC checks. Data include the average absolute difference between duplicate measurements  $\pm 1\sigma$  stdev for each parameter. Also shown are the mean calculated residuals (measured – calculated)  $\pm 3\sigma$  stdev threshold values for each parameter subsetted by input pair used in the calculations.

| Parameter                                 | Measurements:<br>Avg. duplicate difference<br>$\pm 1\sigma$ stdev | Calculations:<br>Mean residual<br>$\pm 3\sigma$ stdev   |
|---|---|---|
| TA<br>( $\mu\text{mol kg}^{-1}$ )         | $1.0 \pm 0.8$<br>( $n = 124$ )                                    | DIC, $\text{pH}_T(25)$ : $0 \pm 12$<br>DIC, $f\text{CO}_2(20)$ : $-10 \pm 12$                     |
| DIC<br>( $\mu\text{mol kg}^{-1}$ )        | $1.8 \pm 1.4$<br>( $n = 168$ )                                    | TA, $\text{pH}_T(25)$ : $0 \pm 12$<br>TA, $f\text{CO}_2(20)$ : $8 \pm 11$                         |
| $\text{pH}_T(25)$                         | $0.0013 \pm 0.0013$<br>( $n = 145$ )                              | TA, $f\text{CO}_2(20)$ and DIC, $f\text{CO}_2(20)$ : $-0.02 \pm 0.01$<br>TA, DIC: $0.00 \pm 0.03$ |
| $f\text{CO}_2(20)$<br>( $\mu\text{atm}$ ) | $0.5 \pm 0.3$<br>( $n = 75$ )                                     | TA, $\text{pH}_T(25)$ and DIC, $\text{pH}_T(25)$ : $-5\% \pm 3\%$<br>TA, DIC: $-5\% \pm 7\%$      |

Residuals of TA, DIC,  $\text{pH}_T(25)$ , and  $f\text{CO}_2(20)$  were calculated with the full dataset using all available sets of input pairs. The mean residuals  $\pm 3\sigma$  stdev for residuals calculated using various sets of input pairs are provided in Table 7. These mean residuals  $\pm 3\sigma$  stdev values were used as a quantitative threshold for quality control purposes. Any residual greater than  $3\sigma$  from the mean residual value was flagged for further analysis. In contrast to the A16N 2023 Leg 1 residuals (Schockman, 2025), the residuals calculated for A16N 2023 Leg 2 were more dissimilar for a single parameter depending on which set of input parameters was used (e.g., the mean residual  $\pm 3\sigma$  stdev thresholds for TA calculated using (DIC,  $\text{pH}_T(25)$ ) and (DIC,  $f\text{CO}_2(20)$ ) were different; see Table 7). Therefore, the mean residual  $\pm 3\sigma$  stdev values were individually calculated specific to the input pairs used and these respective thresholds were implemented during the flagging

process. A list of samples was collated based on these residual flagging guidelines and sent to each of the responsible PIs for additional inspection. Also included in the list were sample points originally flagged as 3 or 4 onboard, but had calculated residuals within the thresholds and no visual indications of an outlier. In these cases, the recommendation was for the PI to check the original data to determine if any of these flags should be changed to a 2.

In general, residuals calculated using one temperature independent parameter (i.e., TA or DIC) and one temperature dependent parameter ( $\text{pH}_T(25)$  or  $f\text{CO}_2(20)$ ) were preferred for flagging purposes. Due to the availability of multiple residuals for each inorganic carbon parameter, it was often clear which, if any, of the four parameters was an incorrect value. As an example, for sample ID #1030222,  $\Delta\text{DIC}$  was  $-32.8 \mu\text{mol kg}^{-1}$  using the (TA,  $\text{pH}_T(25)$ ) pair and  $-3.7 \mu\text{mol kg}^{-1}$  using the (TA,  $f\text{CO}_2(20)$ ) pair. Similarly,  $\Delta\text{TA}$  was  $35.0 \mu\text{mol kg}^{-1}$  using the (DIC,  $\text{pH}_T(25)$ ) pair and  $4.4 \mu\text{mol kg}^{-1}$  using the (DIC,  $f\text{CO}_2(20)$ ) pair. Furthermore,  $\Delta\text{pH}_T$  residuals calculated using all input pairs (on the order of  $-0.055$ ) were larger than the  $3\sigma$  stdev threshold. It would be reasonable to state that the  $\text{pH}_T(25)$  value for this sample is likely an outlier, while the TA, DIC, and  $f\text{CO}_2(20)$  measurements are more internally consistent with one another. In this instance, the recommendation would be to flag this  $\text{pH}_T(25)$  sample as a 3 or 4. In cases where multiple residuals for an individual sample were high and it was unclear which parameter may be incorrect, additional data and visual identification were used for further inspection.

All points visually identified as outliers in the depth profiles of TA, DIC,  $\text{pH}_T(25)$ , or  $f\text{CO}_2(20)$  were included in the list of sample points sent to PIs for additional inspection. Depth profiles of CTD sensor  $\text{O}_2$  and discrete  $\text{O}_2$  were used to determine if a Niskin bottle had been misfired at an incorrect depth and/or if a Niskin bottle had leaked. Comparisons of CTD sensor  $S_p$  and discrete  $S_p$  were also used as a secondary check for Niskin bottle issues. The sampling log

sheets and CTD console log sheets were checked for any reported issues at the time of the CTD cast and/or sampling during the cruise. The combination of depth profile and log sheet checks was used to assign Niskin bottle flags for each sample to be included in the full dataset on CCHDO.

Overall, the recommendations for flag changes were assembled and sent to each of the PIs/parameter leads who checked the data points and had the ultimate say for which (if any) flags should be changed. The number of recommended flag changes and the percentage of these flag changes accepted for each parameter are provided in Table 8. In some cases, the PIs/parameter leads concluded that a flagged parameter value in question was incorrect, and an updated value was provided in lieu of changing the flag designation (these values were still counted as “accepted flag changes” in Table 8). Once the data values and flags were updated, the final inorganic carbon data were submitted to CCHDO to be included with the full cruise dataset.

**Table 8**

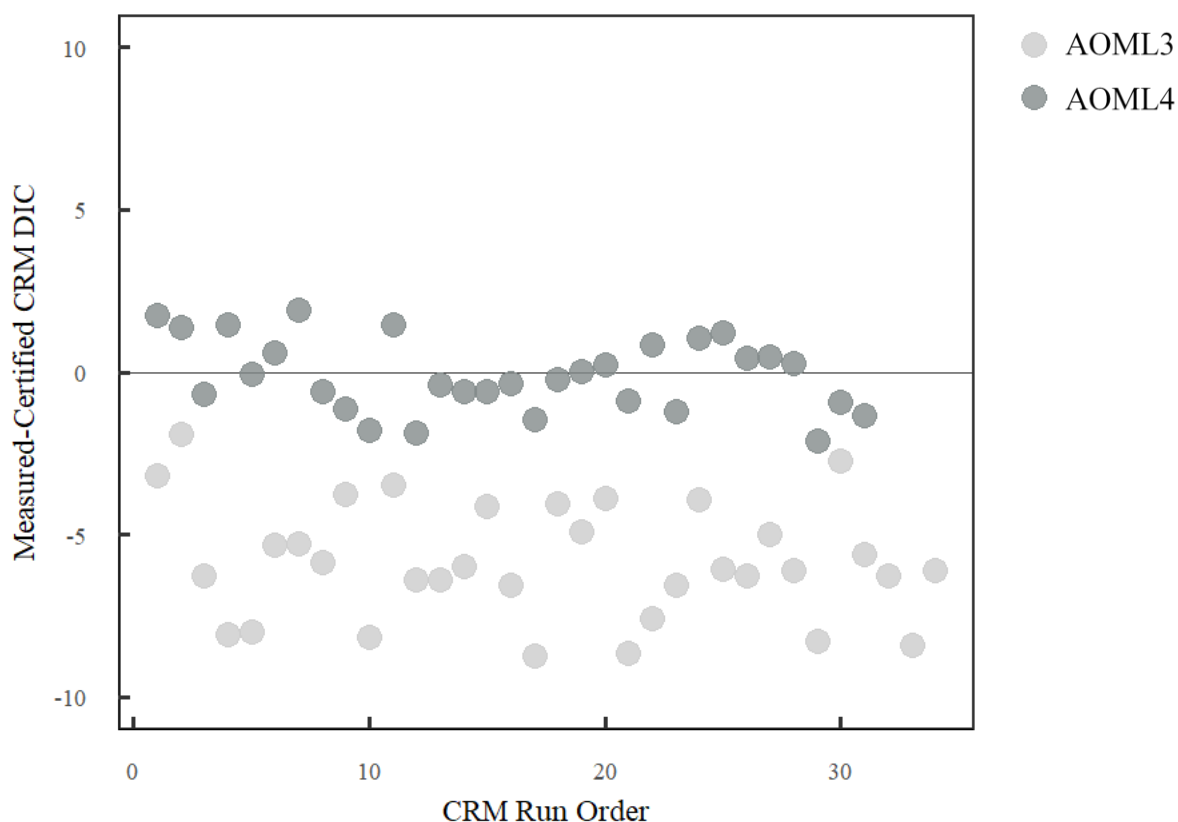
The number of flag changes recommended to each inorganic carbon PI and the number of flag changes accepted (both as a number and as a percentage of the total recommended).

| Parameter             | Recommended<br>flag changes | Accepted<br>flag changes | Percentage of recommended<br>flag changes accepted |
|-----------------------|-----------------------------|--------------------------|--|
| TA                    | 2                           | 2                        | 100%   |
| DIC                   | 2                           | 2                        | 100%   |
| pH <sub>T</sub> (25)  | 10                          | 11                       | 91%  |
| fCO <sub>2</sub> (20) | 4                           | 4                        | 100%   |

### 3.2 CRM Checks Throughout the Cruise

For A16N 2023 Leg 2 DIC measurements, 65 CRMs were run on two identical systems denoted as AOML3 ( $n = 34$ ) and AOML4 ( $n = 31$ ). The average absolute difference between the measured CRM DIC and certified CRM DIC values was  $5.8 \pm 1.8 \mu\text{mol kg}^{-1}$  ( $1\sigma$ ) for AOML3 and  $0.9 \pm 0.6 \mu\text{mol kg}^{-1}$  ( $1\sigma$ ) for AOML4. The differences between measured CRM DIC and certified

CRM DIC values remained generally constant throughout time for both systems, though the differences encompassed a wider range for the AOML3 system compared to the AOML4 system (Fig. 2). The AOML3 system had differences that were consistently negative (i.e., measured CRM DIC was consistently lower than certified CRM DIC), while the AOML4 system differences were evenly distributed about zero. For additional details regarding CRM usage for HCl standardization in TA measurements, please reach out to the individual PI (Table 1).



**Fig. 2.** Differences between measured CRM DIC and certified CRM DIC values shown in terms of the order the CRMs were measured (i.e., throughout the duration of the cruise). As specified above, each difference value between the measured CRM DIC and certified CRM DIC was used to adjust the corresponding subset of measurements for that titration cell, which was replaced approximately every 12 hours. Color denotes the DIC system (AOML3 or AOML4) that corresponds to the CRM measurement.

### 3.3 CO<sub>2</sub>-System Internal Consistency

Internal consistency assessments shown below were made using the final dataset of inorganic carbon parameters on CCHDO after PI flag changes were incorporated (<https://cchdo.ucsd.edu/cruise/33RO20230413>). Residuals were calculated for all samples where

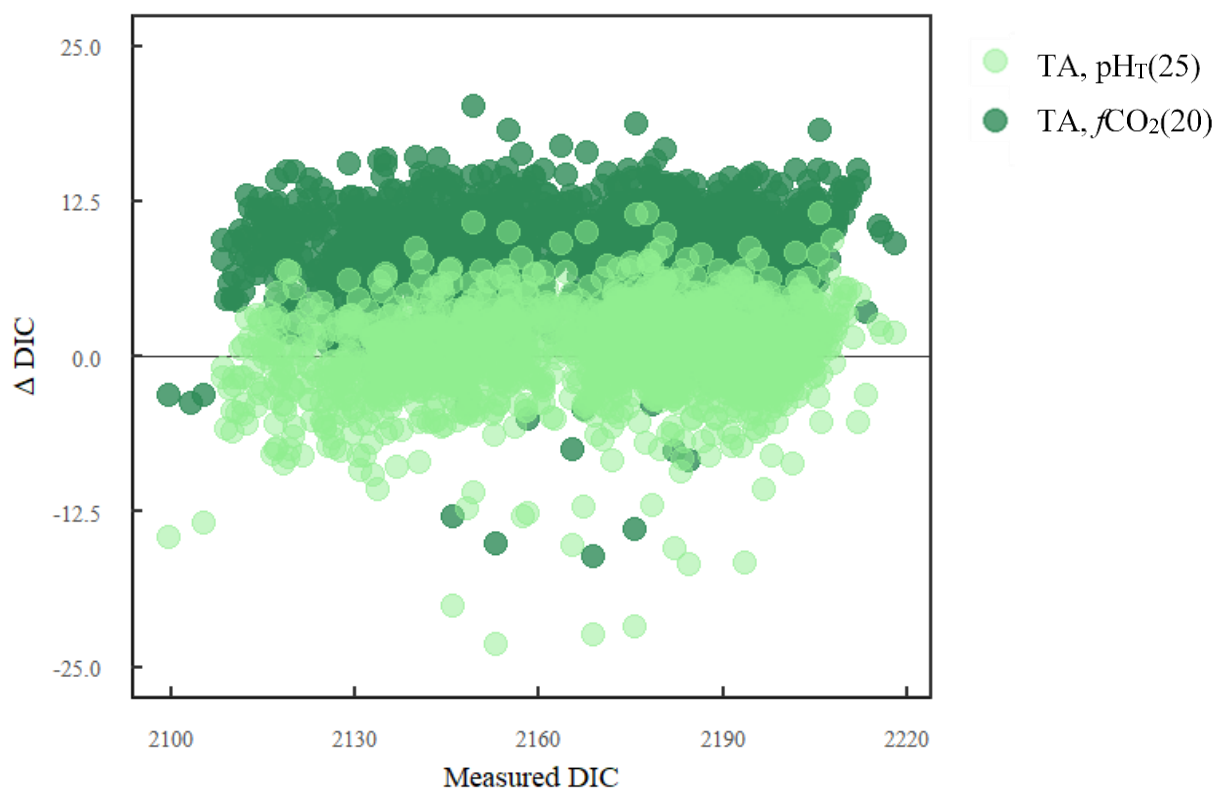
at least three or more inorganic carbon parameters were measured using all available sets of input parameters. Only data with good (2) or duplicate (6) data flags were used for these final internal consistency assessments. (Initial internal consistency assessments were used as a means of secondary QC as described above. However, the data ultimately determined to be questionable (3) or bad (4) quality were removed from this final assessment.)

Residuals of TA and DIC (denoted as  $\Delta\text{TA}$  and  $\Delta\text{DIC}$ ) are generally evenly distributed for the full range of measured TA and DIC (Figs. 3 and 4). For calculations of both TA and DIC, residuals calculated using  $f\text{CO}_2(20)$  as one of the input parameters are in general further from zero compared to residuals calculated using  $\text{pH}_\text{T}(25)$  as one of the input parameters. The offsets observed in the TA and DIC residuals calculated using  $f\text{CO}_2(20)$  appear to be more pronounced than the A16N 2023 Leg 1 TA and DIC residuals calculated in the same manner (Schockman, 2025). In contrast, the TA and DIC residuals calculated using  $\text{pH}_\text{T}(25)$  are evenly distributed about zero for both A16N 2023 Leg 1 and Leg 2.  $\Delta\text{TA}$  and  $\Delta\text{DIC}$  values calculated using the ( $\text{pH}_\text{T}(25)$ ,  $f\text{CO}_2(20)$ ) input pair are not shown as they are larger in magnitude and not recommended according to best practices (Patsavas et al., 2015).





**Fig. 3.** Residuals of TA ( $\Delta TA = \text{measured TA} - \text{calculated TA}$ ;  $\mu\text{mol kg}^{-1}$ ) shown in terms of measured TA. Color denotes the input pair used for TA calculations: (DIC,  $pH_T(25)$ ) or (DIC,  $fCO_2(20)$ ).

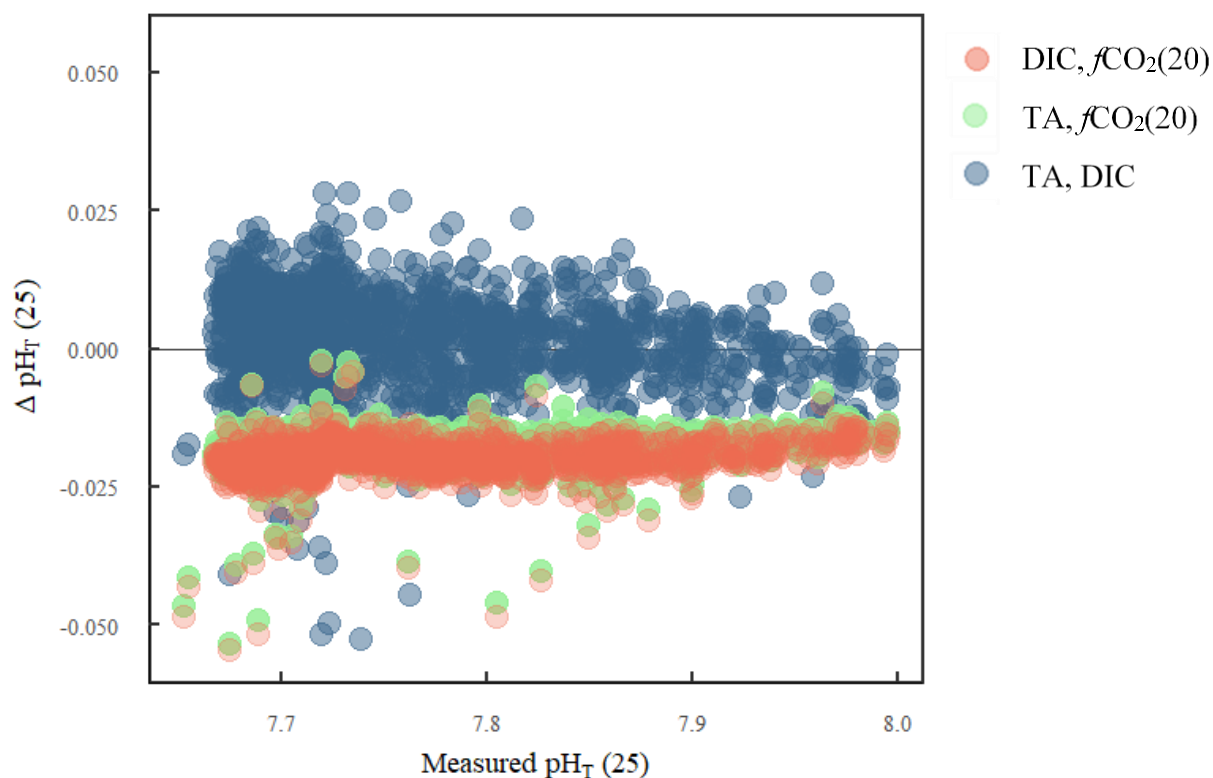


**Fig. 4.** Residuals of DIC ( $\Delta\text{DIC} = \text{measured DIC} - \text{calculated DIC}$ ;  $\mu\text{mol kg}^{-1}$ ) shown in terms of measured DIC. Color denotes the input pair used for DIC calculations: (TA,  $\text{pH}_T(25)$ ) or (TA,  $f\text{CO}_2(20)$ ).

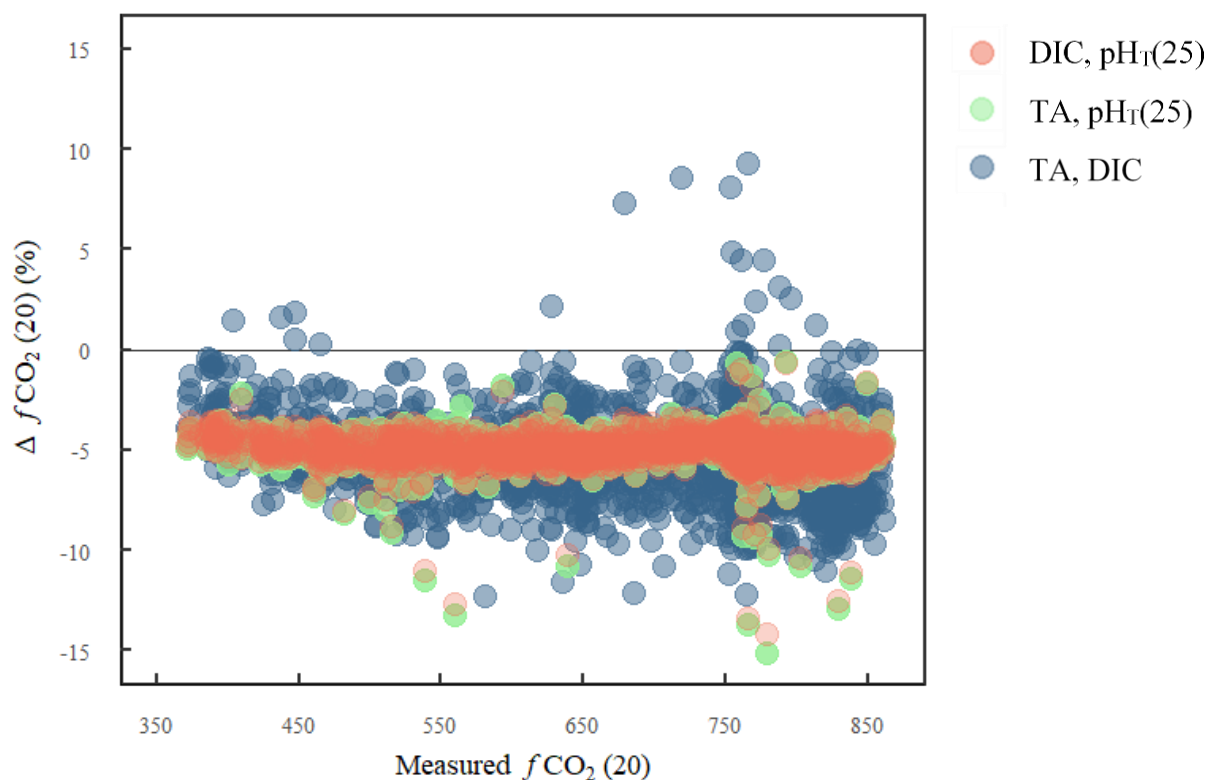
Residuals of  $\text{pH}_T(25)$  (denoted as  $\Delta\text{pH}_T(25)$ ) generally show an even distribution of residuals for the full range of measured  $\text{pH}_T(25)$  (Fig. 5).  $\Delta\text{pH}_T(25)$  values calculated using the (TA, DIC) input pair encompass a larger magnitude than  $\Delta\text{pH}_T(25)$  values calculated using (DIC,  $f\text{CO}_2(20)$ ) and (TA,  $f\text{CO}_2(20)$ ). This finding is expected as it is generally recommended to pair one temperature-independent parameter (i.e., TA or DIC) with one temperature-dependent parameter (i.e.,  $\text{pH}_T(25)$  or  $f\text{CO}_2(20)$ ) in calculations.  $\Delta\text{pH}_T(25)$  values calculated using the (TA, DIC) input pair are generally evenly spread about zero for the full range of measured  $\text{pH}_T(25)$  with no apparent

slope. Similar to A16N 2023 Leg 1 (Schockman, 2025), the previously reported pH-dependent pH offset detected between measured pH and pH(TA, DIC) in many large-scale, oceanographic datasets (McElligott et al., 1998; Williams et al., 2017) is not observed for A16N 2023 Leg 2 data.  $\Delta\text{pH}_T(25)$  values calculated using both (DIC,  $f\text{CO}_2(20)$ ) and (TA,  $f\text{CO}_2(20)$ ) are evenly distributed for the full range of measured  $\text{pH}_T(25)$  though there is a consistent, negative offset in the residual values. This finding suggests that calculated  $\text{pH}_T(25)$  values using  $f\text{CO}_2(20)$  as one of the input parameters are consistently overestimated compared to the respective measured  $\text{pH}_T(25)$  values. The negative offsets in  $\text{pH}_T(25)$  residuals calculated using  $f\text{CO}_2(20)$  appear to be larger in magnitude for the A16N 2023 Leg 2 data compared to Leg 1 data. A piece of equipment for  $f\text{CO}_2(20)$  measurements was replaced between A16N 2023 Leg 1 and Leg 2 (see Section 2.1), which may be responsible for these observed differences.

Residuals of  $f\text{CO}_2(20)$  as a percentage of measured  $f\text{CO}_2(20)$  (denoted as  $\Delta f\text{CO}_2(20)$  (%)) generally show an even distribution of residuals for the full range of measured  $f\text{CO}_2(20)$  (Fig. 6).  $\Delta f\text{CO}_2(20)$  (%) values calculated using all three sets of input pairs have a consistent, negative offset in the residual values. The negative offsets in  $f\text{CO}_2(20)$  (%) residuals appear to be larger in magnitude for the A16N 2023 Leg 2 data compared to Leg 1 data. As mentioned above,  $f\text{CO}_2(20)$  measurement equipment was replaced between Leg 1 and Leg 2, which may be responsible for these observed differences. Similar to  $\Delta\text{pH}_T(25)$  (TA, DIC),  $\Delta f\text{CO}_2(20)$  (%) values calculated using the (TA, DIC) input pair encompass a larger magnitude than  $\Delta f\text{CO}_2(20)$  (%) values calculated using (DIC,  $\text{pH}_T(25)$ ) and (TA,  $\text{pH}_T(25)$ ), which is an expected observation.



**Fig. 5.** Residuals of  $\text{pH}_T(25)$  ( $\Delta \text{pH}_T(25) = \text{measured } \text{pH}_T(25) - \text{calculated } \text{pH}_T(25)$ ) shown in terms of measured  $\text{pH}_T(25)$ . Color denotes the input pair used for  $\text{pH}_T(25)$  calculations: (DIC,  $f\text{CO}_2(20)$ ), (TA,  $f\text{CO}_2(20)$ ), or (TA, DIC). Note that the (DIC,  $f\text{CO}_2(20)$ ) and (TA,  $f\text{CO}_2(20)$ ) points overlap such that (TA,  $f\text{CO}_2(20)$ ) symbols are masked.



**Fig. 6.** Residuals of  $f\text{CO}_2(20)$  as a percentage of measured  $f\text{CO}_2(20)$  ( $\Delta f\text{CO}_2(20) (\%) = (\text{measured } f\text{CO}_2(20) - \text{calculated } f\text{CO}_2(20)) / \text{measured } f\text{CO}_2(20) * 100$ ) shown in terms of measured  $f\text{CO}_2(20)$ . Color denotes the input pair used for  $f\text{CO}_2(20)$  calculations: (DIC,  $\text{pH}_T(25)$ ), (TA,  $\text{pH}_T(25)$ ), or (TA, DIC). Note that the (DIC,  $\text{pH}_T(25)$ ) and (TA,  $\text{pH}_T(25)$ ) points overlap such that (TA,  $\text{pH}_T(25)$ ) symbols are masked.

## 4. Conclusions

This report highlights and describes the quality control measures of the inorganic carbon parameters for the A16N 2023 Leg 2 dataset. The full cruise report located on CCHDO's website contains additional information regarding measurement details and techniques. In general, the inorganic carbon system measurements appear to be of the highest quality standard expected of

GO-SHIP cruises. Like A16N 2023 Leg 1 (Schockman, 2025), Leg 2 also contains measurements of all four inorganic carbon parameters, allowing for a more thorough internal consistency analysis with multiple sets of calculations for each parameter. An important observation is the systematic offset observed when using  $f\text{CO}_2(20)$  as an input parameter for calculations, and the corresponding offset between measured and calculated  $f\text{CO}_2(20)$  values. Several reasons for these differences, including known inconsistencies in the inorganic carbon system calculations, have been described elsewhere (Woosley and Moon, 2023; Schockman et al., 2024; Schockman, 2025). Similar to A16N 2023 Leg 1, the offsets in  $f\text{CO}_2(20)$  are presented as a relative (%) difference with larger absolute differences at higher  $f\text{CO}_2(20)$  values that could be caused by analytical issues, in particular loss of  $\text{CO}_2$  from the headspace during analysis. However, no such issue is apparent in laboratory tests. The internal consistency assessments described here and the notable discrepancies between measured and calculated  $f\text{CO}_2(20)$  further highlight the need for more routine measurements of  $f\text{CO}_2(20)$  to conduct these types of comparisons.

## 5. Additional Tables

**Table 3**

Individual duplicate measurement values of TA ( $\mu\text{mol kg}^{-1}$ ; duplicate one and duplicate two), measured back-to-back, as well as the absolute difference between duplicates. Measurements are provided according to their sample ID.

| Sample ID | TA:<br>Duplicate One | TA:<br>Duplicate Two | Absolute<br>Difference |
|-----------|----------------------|----------------------|------------------------|
| 760102    | 2349.03              | 2346.26              | 2.77                   |
| 760123    | 2433.78              | 2436.25              | 2.47                   |
| 770118    | 2346.98              | 2347.52              | 0.54                   |
| 780209    | 2325.98              | 2325.39              | 0.59                   |
| 780223    | 2427.00              | 2426.85              | 0.15                   |
| 790107    | 2336.68              | 2336.64              | 0.04                   |
| 790116    | 2354.94              | 2353.29              | 1.65                   |
| 800204    | 2340.99              | 2342.05              | 1.06                   |
| 800220    | 2389.94              | 2390.83              | 0.89                   |
| 810111    | 2324.46              | 2323.42              | 1.04                   |
| 810123    | 2420.99              | 2421.13              | 0.14                   |
| 820104    | 2342.79              | 2343.10              | 0.31                   |
| 820121    | 2395.40              | 2396.82              | 1.42                   |
| 830203    | 2342.92              | 2342.44              | 0.48                   |
| 830215    | 2343.11              | 2344.21              | 1.10                   |
| 840106    | 2337.68              | 2337.97              | 0.29                   |
| 840120    | 2372.29              | 2370.00              | 2.29                   |
| 850107    | 2337.19              | 2335.71              | 1.48                   |
| 850116    | 2334.91              | 2336.53              | 1.62                   |
| 860104    | 2340.60              | 2340.34              | 0.26                   |
| 860111    | 2319.61              | 2319.71              | 0.10                   |
| 870109    | 2319.88              | 2319.87              | 0.01                   |
| 870120    | 2371.78              | 2372.37              | 0.59                   |
| 880113    | 2328.35              | 2327.57              | 0.78                   |
| 880116    | 2335.50              | 2335.61              | 0.11                   |
| 890206    | 2337.06              | 2338.00              | 0.94                   |
| 890213    | 2326.11              | 2327.71              | 1.60                   |
| 900113    | 2337.22              | 2338.52              | 1.30                   |
| 900122    | 2377.32              | 2378.05              | 0.73                   |
| 910104    | 2342.44              | 2340.86              | 1.58                   |
| 910112    | 2319.59              | 2318.15              | 1.44                   |
| 920309    | 2322.70              | 2322.36              | 0.34                   |
| 920314    | 2355.96              | 2356.28              | 0.32                   |
| 930113    | 2341.01              | 2343.10              | 2.09                   |
| 930119    | 2343.36              | 2342.16              | 1.20                   |
| 940103    | 2332.56              | 2333.09              | 0.53                   |

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|         |         |         |      |
|---------|---------|---------|------|
| 940117  | 2356.11 | 2356.61 | 0.50 |
| 950205  | 2336.69 | 2337.20 | 0.51 |
| 950216  | 2334.59 | 2334.31 | 0.28 |
| 960306  | 2333.33 | 2332.83 | 0.50 |
| 960315  | 2326.84 | 2330.11 | 3.27 |
| 970109  | 2357.87 | 2358.94 | 1.07 |
| 970119  | 2360.26 | 2359.61 | 0.65 |
| 980206  | 2317.18 | 2315.85 | 1.33 |
| 980213  | 2343.51 | 2345.23 | 1.72 |
| 990218  | 2347.82 | 2347.46 | 0.36 |
| 990223  | 2361.16 | 2362.94 | 1.78 |
| 1000108 | 2308.71 | 2308.41 | 0.30 |
| 1000117 | 2348.81 | 2349.18 | 0.37 |
| 1010105 | 2331.13 | 2331.00 | 0.13 |
| 1010111 | 2352.84 | 2351.11 | 1.73 |
| 1020110 | 2349.63 | 2348.10 | 1.53 |
| 1020121 | 2356.19 | 2357.20 | 1.01 |
| 1030205 | 2333.07 | 2334.45 | 1.38 |
| 1030220 | 2353.62 | 2353.92 | 0.30 |
| 1040102 | 2308.44 | 2305.27 | 3.17 |
| 1040113 | 2339.59 | 2339.88 | 0.29 |
| 1050105 | 2307.56 | 2308.30 | 0.74 |
| 1050116 | 2345.29 | 2343.74 | 1.55 |
| 1060114 | 2331.01 | 2331.10 | 0.09 |
| 1060119 | 2345.53 | 2344.89 | 0.64 |
| 1070106 | 2308.20 | 2308.62 | 0.42 |
| 1070116 | 2337.93 | 2339.64 | 1.71 |
| 1080203 | 2329.16 | 2330.27 | 1.11 |
| 1080214 | 2336.52 | 2335.09 | 1.43 |
| 1090102 | 2346.19 | 2346.28 | 0.09 |
| 1090123 | 2348.14 | 2347.71 | 0.43 |
| 1100107 | 2300.72 | 2301.98 | 1.26 |
| 1100119 | 2348.77 | 2346.36 | 2.41 |
| 1110103 | 2339.14 | 2338.84 | 0.30 |
| 1110118 | 2346.65 | 2346.90 | 0.25 |
| 1120210 | 2306.48 | 2306.75 | 0.27 |
| 1120220 | 2347.68 | 2347.96 | 0.28 |
| 1130108 | 2303.25 | 2300.22 | 3.03 |
| 1130117 | 2338.86 | 2336.98 | 1.88 |
| 1140104 | 2338.38 | 2337.60 | 0.78 |
| 1140121 | 2347.72 | 2345.38 | 2.34 |
| 1150109 | 2298.48 | 2299.22 | 0.74 |
| 1150116 | 2330.55 | 2330.38 | 0.17 |
| 1160113 | 2320.62 | 2321.21 | 0.59 |

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|         |         |         |      |
|---------|---------|---------|------|
| 1160121 | 2345.44 | 2347.33 | 1.89 |
| 1170109 | 2313.66 | 2312.70 | 0.96 |
| 1170113 | 2318.87 | 2318.91 | 0.04 |
| 1180104 | 2333.01 | 2333.20 | 0.19 |
| 1180119 | 2334.65 | 2336.39 | 1.74 |
| 1190106 | 2298.92 | 2298.70 | 0.22 |
| 1190121 | 2335.90 | 2336.87 | 0.97 |
| 1200108 | 2298.80 | 2299.65 | 0.85 |
| 1200112 | 2323.85 | 2324.30 | 0.45 |
| 1210110 | 2307.85 | 2309.48 | 1.63 |
| 1210118 | 2322.14 | 2324.77 | 2.63 |
| 1220105 | 2303.13 | 2304.03 | 0.90 |
| 1220115 | 2314.06 | 2314.87 | 0.81 |
| 1230202 | 2347.65 | 2348.68 | 1.03 |
| 1230217 | 2317.74 | 2316.19 | 1.55 |
| 1240109 | 2302.21 | 2303.93 | 1.72 |
| 1240119 | 2328.67 | 2327.54 | 1.13 |
| 1250103 | 2300.28 | 2300.51 | 0.23 |
| 1250123 | 2334.81 | 2333.56 | 1.25 |
| 1260206 | 2300.92 | 2301.60 | 0.68 |
| 1260214 | 2324.38 | 2324.93 | 0.55 |
| 1270110 | 2311.90 | 2313.68 | 1.78 |
| 1270118 | 2322.18 | 2322.54 | 0.36 |
| 1280103 | 2311.01 | 2311.64 | 0.63 |
| 1280113 | 2328.66 | 2329.39 | 0.73 |
| 1290105 | 2318.88 | 2318.94 | 0.06 |
| 1290114 | 2327.13 | 2328.54 | 1.41 |
| 1300117 | 2314.00 | 2314.60 | 0.60 |
| 1310221 | 2319.79 | 2318.13 | 1.66 |
| 1340111 | 2328.50 | 2326.60 | 1.90 |
| 1340115 | 2325.58 | 2324.12 | 1.46 |
| 1350117 | 2318.22 | 2320.42 | 2.20 |
| 1360103 | 2301.56 | 2301.87 | 0.31 |
| 1360119 | 2322.03 | 2323.82 | 1.79 |
| 1370112 | 2312.05 | 2310.71 | 1.34 |
| 1380208 | 2302.84 | 2300.36 | 2.48 |
| 1380222 | 2322.25 | 2320.70 | 1.55 |
| 1390104 | 2297.81 | 2300.10 | 2.29 |
| 1390114 | 2317.81 | 2318.10 | 0.29 |
| 1400210 | 2309.62 | 2309.72 | 0.10 |
| 1400217 | 2320.05 | 2321.06 | 1.01 |
| 1420112 | 2312.17 | 2312.62 | 0.45 |
| 1420119 | 2318.93 | 2319.04 | 0.11 |
| 1450207 | 2310.81 | 2309.10 | 1.71 |

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**Table 4**

Individual duplicate measurement values of DIC ( $\mu\text{mol kg}^{-1}$ ; duplicate one and duplicate two), measured randomly throughout a cell run, as well as the absolute difference between duplicates. Also included is the system on which each set of duplicates was run (AOML3 or AOML4). Measurements are provided according to their sample ID.

| Sample ID | DIC:<br>Duplicate One | DIC:<br>Duplicate Two | Absolute<br>Difference | System |
|-----------|-----------------------|-----------------------|------------------------|--------|
| 760101    | 2201.89               | 2202.22               | 0.34                   | AOML4  |
| 760115    | 2166.64               | 2170.68               | 4.04                   | AOML4  |
| 760124    | 2131.83               | 2132.24               | 0.40                   | AOML4  |
| 770101    | 2200.39               | 2196.74               | 3.65                   | AOML3  |
| 770117    | 2172.05               | 2173.79               | 1.74                   | AOML3  |
| 770124    | 2127.06               | 2127.66               | 0.59                   | AOML3  |
| 780216    | 2191.18               | 2190.47               | 0.71                   | AOML4  |
| 780224    | 2140.55               | 2136.42               | 4.13                   | AOML4  |
| 790102    | 2196.76               | 2199.41               | 2.65                   | AOML3  |
| 790117    | 2170.17               | 2173.16               | 2.99                   | AOML3  |
| 790124    | 2129.13               | 2123.82               | 5.32                   | AOML3  |
| 800202    | 2197.61               | 2197.20               | 0.41                   | AOML4  |
| 800215    | 2196.03               | 2196.83               | 0.80                   | AOML4  |
| 800224    | 2132.54               | 2130.62               | 1.92                   | AOML4  |
| 810102    | 2200.16               | 2202.34               | 2.18                   | AOML3  |
| 810116    | 2191.07               | 2195.96               | 4.89                   | AOML3  |
| 810124    | 2133.40               | 2133.72               | 0.33                   | AOML3  |
| 820102    | 2199.86               | 2200.85               | 0.99                   | AOML4  |
| 820116    | 2186.50               | 2189.91               | 3.41                   | AOML4  |
| 820124    | 2127.02               | 2125.33               | 1.69                   | AOML4  |
| 830216    | 2186.41               | 2190.48               | 4.07                   | AOML3  |
| 830224    | 2125.60               | 2124.85               | 0.75                   | AOML3  |
| 840103    | 2200.01               | 2202.43               | 2.41                   | AOML4  |
| 840114    | 2205.66               | 2207.05               | 1.39                   | AOML4  |
| 850102    | 2198.49               | 2201.95               | 3.46                   | AOML3  |
| 850115    | 2197.39               | 2203.19               | 5.80                   | AOML3  |
| 850124    | 2135.36               | 2130.82               | 4.54                   | AOML3  |
| 860116    | 2183.94               | 2186.02               | 2.07                   | AOML4  |
| 860124    | 2118.65               | 2118.36               | 0.29                   | AOML4  |
| 870102    | 2198.69               | 2201.94               | 3.25                   | AOML3  |
| 870116    | 2183.99               | 2184.40               | 0.41                   | AOML3  |
| 870123    | 2120.87               | 2119.25               | 1.62                   | AOML3  |
| 880102    | 2201.64               | 2199.69               | 1.95                   | AOML4  |
| 880117    | 2168.05               | 2169.26               | 1.20                   | AOML4  |
| 880124    | 2125.62               | 2123.97               | 1.65                   | AOML4  |
| 890201    | 2204.61               | 2202.84               | 1.77                   | AOML3  |
| 890215    | 2201.93               | 2201.66               | 0.27                   | AOML3  |

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|         |         |         |      |       |
|---------|---------|---------|------|-------|
| 890222  | 2117.40 | 2118.86 | 1.46 | AOML3 |
| 900101  | 2202.68 | 2205.10 | 2.42 | AOML4 |
| 900115  | 2198.79 | 2199.43 | 0.64 | AOML4 |
| 900124  | 2119.60 | 2121.38 | 1.79 | AOML4 |
| 910101  | 2201.60 | 2203.62 | 2.02 | AOML3 |
| 910117  | 2173.03 | 2171.61 | 1.42 | AOML3 |
| 920301  | 2204.06 | 2202.09 | 1.97 | AOML4 |
| 920316  | 2194.41 | 2193.97 | 0.44 | AOML4 |
| 920321  | 2138.52 | 2139.85 | 1.32 | AOML4 |
| 930102  | 2202.54 | 2205.62 | 3.08 | AOML3 |
| 930115  | 2203.62 | 2203.00 | 0.61 | AOML3 |
| 930123  | 2119.35 | 2123.25 | 3.89 | AOML3 |
| 940102  | 2198.26 | 2201.08 | 2.82 | AOML4 |
| 940112  | 2190.88 | 2191.98 | 1.10 | AOML4 |
| 940124  | 2122.70 | 2120.65 | 2.06 | AOML4 |
| 950201  | 2202.22 | 2202.32 | 0.10 | AOML3 |
| 950211  | 2200.73 | 2203.24 | 2.51 | AOML3 |
| 950224  | 2110.70 | 2108.30 | 2.40 | AOML3 |
| 960302  | 2199.31 | 2203.39 | 4.08 | AOML4 |
| 960314  | 2183.08 | 2182.21 | 0.86 | AOML4 |
| 960324  | 2110.05 | 2113.34 | 3.29 | AOML4 |
| 970101  | 2201.02 | 2200.48 | 0.53 | AOML3 |
| 970110  | 2205.03 | 2201.97 | 3.06 | AOML3 |
| 970124  | 2107.59 | 2112.01 | 4.42 | AOML3 |
| 980201  | 2206.65 | 2205.51 | 1.14 | AOML4 |
| 980212  | 2199.85 | 2200.33 | 0.47 | AOML4 |
| 990201  | 2205.68 | 2205.57 | 0.11 | AOML3 |
| 990212  | 2205.06 | 2205.07 | 0.01 | AOML3 |
| 990224  | 2112.48 | 2113.07 | 0.59 | AOML3 |
| 1000102 | 2199.20 | 2201.97 | 2.77 | AOML4 |
| 1000112 | 2192.70 | 2194.36 | 1.67 | AOML4 |
| 1000124 | 2110.73 | 2111.47 | 0.74 | AOML4 |
| 1010102 | 2200.66 | 2200.51 | 0.14 | AOML3 |
| 1010113 | 2192.37 | 2190.04 | 2.32 | AOML3 |
| 1010124 | 2111.24 | 2105.44 | 5.80 | AOML3 |
| 1020102 | 2203.55 | 2204.13 | 0.58 | AOML4 |
| 1020124 | 2113.03 | 2115.72 | 2.70 | AOML4 |
| 1030202 | 2172.21 | 2170.31 | 1.90 | AOML3 |
| 1030224 | 2103.02 | 2095.74 | 7.28 | AOML3 |
| 1040103 | 2171.99 | 2171.14 | 0.86 | AOML4 |
| 1040112 | 2162.55 | 2161.52 | 1.04 | AOML4 |
| 1040124 | 2112.99 | 2114.52 | 1.53 | AOML4 |
| 1060101 | 2206.10 | 2209.22 | 3.12 | AOML4 |
| 1060112 | 2201.66 | 2204.52 | 2.86 | AOML4 |

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|         |         |         |      |       |
|---------|---------|---------|------|-------|
| 1060122 | 2133.85 | 2132.04 | 1.81 | AOML4 |
| 1070101 | 2209.16 | 2208.03 | 1.14 | AOML3 |
| 1070111 | 2196.74 | 2195.99 | 0.75 | AOML3 |
| 1070124 | 2115.15 | 2114.57 | 0.58 | AOML3 |
| 1080201 | 2204.90 | 2203.71 | 1.18 | AOML4 |
| 1080211 | 2182.57 | 2183.09 | 0.53 | AOML4 |
| 1080224 | 2110.21 | 2109.93 | 0.28 | AOML4 |
| 1090101 | 2206.86 | 2204.01 | 2.84 | AOML3 |
| 1090112 | 2184.04 | 2184.17 | 0.13 | AOML3 |
| 1090124 | 2113.75 | 2116.22 | 2.48 | AOML3 |
| 1100101 | 2207.86 | 2207.78 | 0.08 | AOML4 |
| 1100111 | 2194.68 | 2192.10 | 2.57 | AOML4 |
| 1100124 | 2116.08 | 2116.60 | 0.51 | AOML4 |
| 1110101 | 2208.32 | 2208.31 | 0.01 | AOML3 |
| 1110112 | 2185.71 | 2188.83 | 3.12 | AOML3 |
| 1110124 | 2115.41 | 2114.25 | 1.16 | AOML3 |
| 1120203 | 2203.59 | 2202.19 | 1.40 | AOML4 |
| 1120214 | 2179.79 | 2177.64 | 2.15 | AOML4 |
| 1120224 | 2114.87 | 2116.63 | 1.76 | AOML4 |
| 1130101 | 2206.99 | 2205.03 | 1.95 | AOML3 |
| 1130113 | 2188.24 | 2192.70 | 4.46 | AOML3 |
| 1130124 | 2117.30 | 2113.64 | 3.66 | AOML3 |
| 1140101 | 2208.49 | 2206.75 | 1.74 | AOML4 |
| 1140112 | 2193.72 | 2190.45 | 3.28 | AOML4 |
| 1140124 | 2112.45 | 2112.07 | 0.38 | AOML4 |
| 1150124 | 2122.66 | 2122.29 | 0.37 | AOML3 |
| 1160101 | 2210.89 | 2209.19 | 1.70 | AOML3 |
| 1160113 | 2184.15 | 2184.55 | 0.41 | AOML3 |
| 1160124 | 2122.11 | 2124.05 | 1.94 | AOML3 |
| 1170101 | 2208.15 | 2208.19 | 0.04 | AOML4 |
| 1170111 | 2195.88 | 2194.93 | 0.95 | AOML4 |
| 1170121 | 2141.59 | 2146.58 | 4.98 | AOML4 |
| 1180101 | 2209.60 | 2210.22 | 0.62 | AOML3 |
| 1180113 | 2186.45 | 2192.89 | 6.44 | AOML3 |
| 1180124 | 2117.96 | 2118.50 | 0.55 | AOML3 |
| 1190112 | 2168.29 | 2167.77 | 0.51 | AOML4 |
| 1190122 | 2116.91 | 2117.07 | 0.15 | AOML4 |
| 1200102 | 2204.32 | 2206.25 | 1.93 | AOML3 |
| 1200113 | 2167.55 | 2166.06 | 1.49 | AOML3 |
| 1200124 | 2124.69 | 2124.18 | 0.51 | AOML3 |
| 1210102 | 2204.34 | 2205.58 | 1.24 | AOML4 |
| 1210113 | 2184.22 | 2185.98 | 1.77 | AOML4 |
| 1210124 | 2126.41 | 2126.46 | 0.06 | AOML4 |
| 1220102 | 2204.42 | 2204.05 | 0.37 | AOML3 |

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|         |         |         |      |       |
|---------|---------|---------|------|-------|
| 1220113 | 2190.59 | 2190.78 | 0.19 | AOML3 |
| 1220124 | 2129.58 | 2128.60 | 0.98 | AOML3 |
| 1230201 | 2209.14 | 2208.10 | 1.04 | AOML4 |
| 1230224 | 2120.11 | 2118.61 | 1.49 | AOML4 |
| 1240101 | 2210.14 | 2208.56 | 1.58 | AOML3 |
| 1240113 | 2188.42 | 2190.25 | 1.83 | AOML3 |
| 1250101 | 2190.12 | 2191.26 | 1.14 | AOML4 |
| 1250124 | 2125.40 | 2123.45 | 1.95 | AOML4 |
| 1260201 | 2193.50 | 2192.97 | 0.53 | AOML3 |
| 1260211 | 2188.92 | 2188.22 | 0.70 | AOML3 |
| 1270101 | 2188.28 | 2187.79 | 0.48 | AOML4 |
| 1270124 | 2115.99 | 2112.86 | 3.14 | AOML4 |
| 1280101 | 2181.85 | 2177.76 | 4.09 | AOML3 |
| 1280121 | 2134.90 | 2132.63 | 2.27 | AOML3 |
| 1290121 | 2119.15 | 2120.19 | 1.04 | AOML4 |
| 1300122 | 2118.77 | 2117.46 | 1.31 | AOML3 |
| 1310224 | 2125.65 | 2127.25 | 1.60 | AOML4 |
| 1320121 | 2124.41 | 2126.87 | 2.46 | AOML3 |
| 1330121 | 2134.68 | 2133.48 | 1.20 | AOML4 |
| 1340117 | 2140.59 | 2139.15 | 1.44 | AOML3 |
| 1350121 | 2139.29 | 2136.56 | 2.73 | AOML4 |
| 1360101 | 2171.74 | 2170.06 | 1.68 | AOML3 |
| 1360124 | 2138.41 | 2139.41 | 1.00 | AOML3 |
| 1370102 | 2173.62 | 2173.05 | 0.57 | AOML4 |
| 1370123 | 2144.25 | 2141.06 | 3.19 | AOML4 |
| 1380201 | 2180.90 | 2180.37 | 0.53 | AOML3 |
| 1380212 | 2182.66 | 2180.68 | 1.97 | AOML3 |
| 1380224 | 2141.83 | 2141.04 | 0.79 | AOML3 |
| 1390102 | 2173.57 | 2175.56 | 1.99 | AOML4 |
| 1390113 | 2169.35 | 2170.66 | 1.31 | AOML4 |
| 1390124 | 2145.61 | 2145.00 | 0.61 | AOML4 |
| 1400201 | 2179.86 | 2175.75 | 4.11 | AOML3 |
| 1400213 | 2154.48 | 2155.09 | 0.61 | AOML3 |
| 1400224 | 2141.25 | 2144.11 | 2.86 | AOML3 |
| 1410101 | 2184.42 | 2185.28 | 0.86 | AOML4 |
| 1410124 | 2150.47 | 2150.18 | 0.28 | AOML4 |
| 1420101 | 2182.03 | 2180.00 | 2.03 | AOML3 |
| 1420109 | 2188.57 | 2190.35 | 1.78 | AOML3 |
| 1420124 | 2150.62 | 2148.82 | 1.80 | AOML3 |
| 1430124 | 2151.77 | 2152.76 | 0.99 | AOML4 |
| 1440124 | 2152.54 | 2153.28 | 0.74 | AOML4 |
| 1450201 | 2176.33 | 2171.19 | 5.14 | AOML3 |
| 1450224 | 2149.20 | 2148.24 | 0.96 | AOML3 |

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**Table 5**

Individual duplicate measurement values of  $\text{pH}_T(25)$  (duplicate one and duplicate two), measured back-to-back, as well as the absolute difference between duplicates. Measurements are provided according to their sample ID.

| Sample ID | $\text{pH}_T(25)$ :<br>Duplicate One | $\text{pH}_T(25)$ :<br>Duplicate Two | Absolute<br>Difference |
|-----------|--------------------------------------|--------------------------------------|------------------------|
| 760102    | 7.7176                               | 7.7221                               | 0.0045                 |
| 760123    | 7.9940                               | 7.9932                               | 0.0008                 |
| 770105    | 7.7217                               | 7.7233                               | 0.0016                 |
| 770118    | 7.8048                               | 7.8043                               | 0.0005                 |
| 780209    | 7.7218                               | 7.7240                               | 0.0022                 |
| 780223    | 7.9813                               | 7.9820                               | 0.0007                 |
| 790107    | 7.7221                               | 7.7221                               | 0.0000                 |
| 790116    | 7.7422                               | 7.7416                               | 0.0006                 |
| 800204    | 7.7214                               | 7.7214                               | 0.0000                 |
| 800220    | 7.9114                               | 7.9105                               | 0.0009                 |
| 810111    | 7.7224                               | 7.7223                               | 0.0000                 |
| 810123    | 7.9797                               | 7.9788                               | 0.0009                 |
| 820104    | 7.7206                               | 7.7207                               | 0.0000                 |
| 820121    | 7.9505                               | 7.9515                               | 0.0010                 |
| 830203    | 7.7220                               | 7.7216                               | 0.0004                 |
| 830215    | 7.7108                               | 7.7195                               | 0.0088                 |
| 840106    | 7.7244                               | 7.7221                               | 0.0023                 |
| 840120    | 7.8863                               | 7.8870                               | 0.0008                 |
| 850107    | 7.7221                               | 7.7222                               | 0.0001                 |
| 850116    | 7.7192                               | 7.7199                               | 0.0007                 |
| 860104    | 7.7217                               | 7.7212                               | 0.0005                 |
| 860111    | 7.7211                               | 7.7216                               | 0.0005                 |
| 870109    | 7.7228                               | 7.7217                               | 0.0011                 |
| 870120    | 7.9048                               | 7.9057                               | 0.0009                 |
| 880113    | 7.7169                               | 7.7165                               | 0.0004                 |
| 880116    | 7.7293                               | 7.7298                               | 0.0005                 |
| 890206    | 7.7189                               | 7.7210                               | 0.0021                 |
| 890213    | 7.7128                               | 7.7132                               | 0.0004                 |
| 900113    | 7.7208                               | 7.7207                               | 0.0001                 |
| 900122    | 7.9322                               | 7.9334                               | 0.0013                 |
| 910104    | 7.7202                               | 7.7211                               | 0.0009                 |
| 910112    | 7.7162                               | 7.7155                               | 0.0006                 |
| 920309    | 7.7219                               | 7.7229                               | 0.0010                 |
| 920314    | 7.7373                               | 7.7392                               | 0.0019                 |
| 930113    | 7.7248                               | 7.7243                               | 0.0005                 |
| 930119    | 7.8124                               | 7.8131                               | 0.0007                 |
| 940103    | 7.7171                               | 7.7154                               | 0.0017                 |
| 940117    | 7.8586                               | 7.8575                               | 0.0011                 |

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|         |        |        |        |
|---------|--------|--------|--------|
| 950205  | 7.7160 | 7.7179 | 0.0019 |
| 950216  | 7.7866 | 7.7874 | 0.0008 |
| 960306  | 7.7182 | 7.7168 | 0.0013 |
| 960315  | 7.7421 | 7.7426 | 0.0005 |
| 970109  | 7.7355 | 7.7363 | 0.0008 |
| 970119  | 7.8822 | 7.8820 | 0.0003 |
| 980206  | 7.7159 | 7.7145 | 0.0014 |
| 980213  | 7.7390 | 7.7390 | 0.0000 |
| 990218  | 7.8458 | 7.8458 | 0.0000 |
| 990223  | 7.9329 | 7.9316 | 0.0013 |
| 1000108 | 7.7026 | 7.7031 | 0.0005 |
| 1000117 | 7.8380 | 7.8396 | 0.0016 |
| 1010105 | 7.7135 | 7.7146 | 0.0011 |
| 1010111 | 7.7278 | 7.7296 | 0.0017 |
| 1020110 | 7.7260 | 7.7248 | 0.0012 |
| 1020121 | 7.9050 | 7.9026 | 0.0024 |
| 1030205 | 7.7146 | 7.7157 | 0.0011 |
| 1030220 | 7.8750 | 7.8750 | 0.0001 |
| 1040102 | 7.7044 | 7.7036 | 0.0008 |
| 1040113 | 7.8060 | 7.8044 | 0.0015 |
| 1050105 | 7.7079 | 7.7070 | 0.0009 |
| 1050116 | 7.8475 | 7.8473 | 0.0002 |
| 1060114 | 7.7315 | 7.7326 | 0.0011 |
| 1060119 | 7.8497 | 7.8497 | 0.0000 |
| 1070106 | 7.7019 | 7.7004 | 0.0015 |
| 1070116 | 7.8011 | 7.7997 | 0.0014 |
| 1080203 | 7.7133 | 7.7129 | 0.0004 |
| 1080214 | 7.8014 | 7.8011 | 0.0003 |
| 1090102 | 7.7206 | 7.7135 | 0.0071 |
| 1090123 | 7.8807 | 7.8824 | 0.0017 |
| 1100107 | 7.6857 | 7.6878 | 0.0021 |
| 1100119 | 7.8597 | 7.8621 | 0.0024 |
| 1110103 | 7.7125 | 7.7127 | 0.0002 |
| 1110118 | 7.8528 | 7.8525 | 0.0003 |
| 1120210 | 7.6838 | 7.6836 | 0.0002 |
| 1120220 | 7.8538 | 7.8568 | 0.0030 |
| 1130108 | 7.6956 | 7.6992 | 0.0036 |
| 1130117 | 7.8266 | 7.8308 | 0.0042 |
| 1140104 | 7.7151 | 7.7144 | 0.0007 |
| 1140121 | 7.8648 | 7.8646 | 0.0003 |
| 1150109 | 7.6865 | 7.6889 | 0.0023 |
| 1150116 | 7.7868 | 7.7827 | 0.0041 |
| 1160113 | 7.7069 | 7.7096 | 0.0027 |
| 1160121 | 7.8653 | 7.8619 | 0.0035 |

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|         |        |        |        |
|---------|--------|--------|--------|
| 1170109 | 7.6904 | 7.6856 | 0.0048 |
| 1170113 | 7.7005 | 7.7007 | 0.0002 |
| 1180104 | 7.7136 | 7.7115 | 0.0020 |
| 1180119 | 7.8235 | 7.8241 | 0.0006 |
| 1190106 | 7.6859 | 7.6852 | 0.0007 |
| 1190121 | 7.8438 | 7.8456 | 0.0018 |
| 1200108 | 7.6812 | 7.6815 | 0.0003 |
| 1200112 | 7.6994 | 7.6978 | 0.0015 |
| 1210110 | 7.6750 | 7.6755 | 0.0005 |
| 1210118 | 7.8005 | 7.7990 | 0.0015 |
| 1220105 | 7.6892 | 7.6889 | 0.0003 |
| 1220115 | 7.7312 | 7.7327 | 0.0016 |
| 1230202 | 7.7160 | 7.7160 | 0.0000 |
| 1230217 | 7.7783 | 7.7781 | 0.0001 |
| 1240109 | 7.6732 | 7.6733 | 0.0002 |
| 1240119 | 7.8077 | 7.8069 | 0.0008 |
| 1250103 | 7.6893 | 7.6867 | 0.0026 |
| 1250123 | 7.8326 | 7.8334 | 0.0008 |
| 1260206 | 7.6780 | 7.6773 | 0.0007 |
| 1260214 | 7.7876 | 7.7866 | 0.0010 |
| 1270110 | 7.6761 | 7.6761 | 0.0001 |
| 1270118 | 7.7963 | 7.7965 | 0.0002 |
| 1280103 | 7.6789 | 7.6780 | 0.0009 |
| 1280113 | 7.8053 | 7.8071 | 0.0018 |
| 1290105 | 7.6807 | 7.6797 | 0.0010 |
| 1290114 | 7.8113 | 7.8068 | 0.0045 |
| 1300117 | 7.7856 | 7.7839 | 0.0017 |
| 1310221 | 7.8054 | 7.8079 | 0.0025 |
| 1320108 | 7.6950 | 7.6956 | 0.0006 |
| 1320114 | 7.7777 | 7.7790 | 0.0013 |
| 1330111 | 7.7945 | 7.7940 | 0.0005 |
| 1330119 | 7.8269 | 7.8250 | 0.0020 |
| 1340111 | 7.8015 | 7.8031 | 0.0016 |
| 1340115 | 7.8094 | 7.8093 | 0.0001 |
| 1350109 | 7.7863 | 7.7873 | 0.0010 |
| 1350117 | 7.8104 | 7.8081 | 0.0023 |
| 1360103 | 7.6754 | 7.6757 | 0.0003 |
| 1360119 | 7.8007 | 7.8008 | 0.0001 |
| 1370112 | 7.6965 | 7.6970 | 0.0005 |
| 1370116 | 7.7560 | 7.7569 | 0.0009 |
| 1380208 | 7.6690 | 7.6693 | 0.0003 |
| 1380222 | 7.7881 | 7.7890 | 0.0009 |
| 1390104 | 7.6842 | 7.6862 | 0.0021 |
| 1390114 | 7.7499 | 7.7516 | 0.0018 |

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|         |        |        |        |
|---------|--------|--------|--------|
| 1400210 | 7.6807 | 7.6801 | 0.0005 |
| 1400217 | 7.7756 | 7.7750 | 0.0006 |
| 1410108 | 7.6715 | 7.6732 | 0.0017 |
| 1410115 | 7.7542 | 7.7552 | 0.0010 |
| 1420112 | 7.7298 | 7.7297 | 0.0001 |
| 1420119 | 7.7739 | 7.7741 | 0.0002 |
| 1430102 | 7.6913 | 7.6914 | 0.0001 |
| 1430122 | 7.7763 | 7.7757 | 0.0006 |
| 1440106 | 7.6684 | 7.6721 | 0.0037 |
| 1440117 | 7.7746 | 7.7733 | 0.0013 |
| 1450207 | 7.6950 | 7.6950 | 0.0001 |
| 1450219 | 7.7707 | 7.7717 | 0.0011 |
| 1470112 | 7.7619 | 7.7596 | 0.0023 |
| 1480111 | 7.7317 | 7.7342 | 0.0025 |
| 1480118 | 7.7741 | 7.7722 | 0.0019 |
| 1490109 | 7.7469 | 7.7461 | 0.0009 |
| 1490113 | 7.7725 | 7.7744 | 0.0019 |
| 1500104 | 7.7442 | 7.7459 | 0.0016 |
| 1500111 | 7.7701 | 7.7713 | 0.0012 |

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**Table 6**

Individual duplicate measurement values of  $f\text{CO}_2(20)$  ( $\mu\text{atm}$ ; duplicate one and duplicate two), measured back-to-back, as well as the absolute and relative differences between duplicates (relative difference = absolute difference / average duplicate value \* 100). Measurements are provided according to their sample ID.

| Sample ID | $f\text{CO}_2(20)$ :<br>Duplicate One | $f\text{CO}_2(20)$ :<br>Duplicate Two | Absolute<br>Difference | Relative<br>Difference (%) |
|-----------|---------------------------------------|---------------------------------------|------------------------|----------------------------|
| 760110    | 826.44                                | 826.79                                | 0.35                   | 0.04                       |
| 770115    | 824.03                                | 825.25                                | 1.22                   | 0.15                       |
| 780206    | 757.77                                | 757.29                                | 0.48                   | 0.06                       |
| 790119    | 518.97                                | 518.18                                | 0.79                   | 0.15                       |
| 800213    | 765.52                                | 765.59                                | 0.07                   | 0.01                       |
| 810103    | 762.17                                | 762.91                                | 0.74                   | 0.10                       |
| 820123    | 388.10                                | 388.98                                | 0.88                   | 0.23                       |
| 830222    | 402.29                                | 402.28                                | 0.01                   | 0.00                       |
| 840109    | 752.13                                | 751.67                                | 0.46                   | 0.06                       |
| 850117    | 697.53                                | 697.12                                | 0.41                   | 0.06                       |
| 860121    | 400.48                                | 400.05                                | 0.43                   | 0.11                       |
| 870119    | 537.99                                | 537.17                                | 0.82                   | 0.15                       |
| 880107    | 759.32                                | 758.98                                | 0.34                   | 0.04                       |
| 890223    | 409.43                                | 409.28                                | 0.15                   | 0.04                       |
| 900111    | 763.85                                | 763.50                                | 0.35                   | 0.05                       |
| 910105    | 759.70                                | 759.34                                | 0.36                   | 0.05                       |
| 920319    | 586.32                                | 585.32                                | 1.00                   | 0.17                       |
| 930108    | 755.35                                | 754.93                                | 0.42                   | 0.06                       |
| 940105    | 755.33                                | 755.46                                | 0.13                   | 0.02                       |
| 950213    | 726.66                                | 726.51                                | 0.15                   | 0.02                       |
| 960322    | 444.88                                | 444.47                                | 0.41                   | 0.09                       |
| 970123    | 428.74                                | 429.00                                | 0.26                   | 0.06                       |
| 980203    | 764.34                                | 764.97                                | 0.63                   | 0.08                       |
| 990214    | 715.07                                | 715.28                                | 0.21                   | 0.03                       |
| 1000103   | 761.92                                | 762.09                                | 0.17                   | 0.02                       |
| 1010107   | 757.75                                | 758.63                                | 0.88                   | 0.12                       |
| 1020119   | 502.30                                | 501.37                                | 0.93                   | 0.19                       |
| 1030212   | 659.85                                | 659.00                                | 0.85                   | 0.13                       |
| 1040109   | 739.59                                | 739.46                                | 0.13                   | 0.02                       |
| 1050106   | 787.71                                | 787.83                                | 0.12                   | 0.02                       |
| 1060111   | 790.96                                | 791.09                                | 0.13                   | 0.02                       |
| 1070119   | 532.02                                | 530.71                                | 1.31                   | 0.25                       |
| 1080205   | 776.18                                | 776.73                                | 0.55                   | 0.07                       |
| 1090109   | 821.00                                | 821.03                                | 0.03                   | 0.00                       |
| 1100117   | 528.59                                | 527.71                                | 0.88                   | 0.17                       |
| 1110105   | 774.59                                | 774.57                                | 0.02                   | 0.00                       |
| 1120222   | 511.95                                | 511.28                                | 0.67                   | 0.13                       |

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|         |        |        |      |      |
|---------|--------|--------|------|------|
| 1130109 | 812.64 | 813.49 | 0.85 | 0.10 |
| 1140113 | 799.69 | 799.25 | 0.44 | 0.06 |
| 1150105 | 770.35 | 770.04 | 0.31 | 0.04 |
| 1160116 | 593.51 | 592.75 | 0.76 | 0.13 |
| 1170104 | 774.98 | 775.66 | 0.68 | 0.09 |
| 1180109 | 829.98 | 830.45 | 0.47 | 0.06 |
| 1190120 | 558.24 | 558.24 | 0.00 | 0.00 |
| 1200110 | 828.82 | 829.13 | 0.31 | 0.04 |
| 1210109 | 841.34 | 840.85 | 0.49 | 0.06 |
| 1220111 | 846.20 | 846.24 | 0.04 | 0.00 |
| 1230206 | 798.50 | 798.70 | 0.20 | 0.03 |
| 1240116 | 637.99 | 636.76 | 1.23 | 0.19 |
| 1250102 | 785.46 | 785.12 | 0.34 | 0.04 |
| 1260203 | 808.06 | 808.20 | 0.14 | 0.02 |
| 1270105 | 819.92 | 819.47 | 0.45 | 0.05 |
| 1280108 | 684.48 | 685.90 | 1.42 | 0.21 |
| 1290106 | 800.64 | 800.08 | 0.56 | 0.07 |
| 1300114 | 624.35 | 624.06 | 0.29 | 0.05 |
| 1310214 | 625.78 | 625.25 | 0.53 | 0.08 |
| 1320118 | 608.28 | 608.37 | 0.09 | 0.01 |
| 1330103 | 838.88 | 838.84 | 0.04 | 0.00 |
| 1340116 | 591.65 | 591.88 | 0.23 | 0.04 |
| 1350103 | 833.55 | 832.93 | 0.62 | 0.07 |
| 1360122 | 600.40 | 600.11 | 0.29 | 0.05 |
| 1370111 | 844.02 | 844.82 | 0.80 | 0.09 |
| 1380207 | 839.45 | 839.81 | 0.36 | 0.04 |
| 1390115 | 670.43 | 670.24 | 0.19 | 0.03 |
| 1400214 | 671.40 | 670.15 | 1.25 | 0.19 |
| 1410123 | 635.20 | 635.83 | 0.63 | 0.10 |
| 1420102 | 794.50 | 794.73 | 0.23 | 0.03 |
| 1430110 | 845.35 | 844.83 | 0.52 | 0.06 |
| 1440118 | 653.28 | 653.17 | 0.11 | 0.02 |
| 1450205 | 812.36 | 812.72 | 0.36 | 0.04 |
| 1460109 | 733.81 | 732.93 | 0.88 | 0.12 |
| 1470103 | 812.61 | 812.09 | 0.52 | 0.06 |
| 1480107 | 771.60 | 771.81 | 0.21 | 0.03 |
| 1490116 | 645.62 | 645.24 | 0.38 | 0.06 |
| 1500106 | 689.81 | 689.66 | 0.15 | 0.02 |

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## 6. References

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