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### Precision analysis and the determination of outliers

Precision was determined by analyzing replicate samples drawn from one Niskin.

Outliers are discarded on the basis of Chauvenet's criteria. The statistic is calculated by finding the Chauvenet critical value (Z-critical) for the total degrees of freedom ( $v$ ) of the dataset:

$$Z\text{-critical} = \text{ABS}(\text{NORM.S.INV}(1/(4*v)))$$

The maximum deviation,  $D_{max}$ , is compared with the individual residuals from the original concentrations.

If a replicate's residual is greater than  $D_{max}$  this value can be rejected.  $D_{max}$  is determined by the following formula:

$$D_{max} = Z\text{-critical} * \sigma$$

where  $\sigma$  is the standard deviation of residuals

Precision is assessed by calculating the pooled standard deviation ( $S_p$ ).

Pooled standard deviation is calculated for a combination of duplicates and triplicates using the following formula:

$$s_p = \sqrt{\frac{SS_1 + SS_2 + \dots + SS_k}{v_1 + v_2 + \dots + v_k}}$$

where:  $v$  = total degrees of freedom (1 for duplicates, 2 for triplicates).

$SS$  = sum of squares of the residuals.

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### Precision statement for replicate samples drawn from a single Niskin bottle:

Salinity: Bottle ranged from 34.3570 to 34.6813 with a pooled standard deviation of 0.0006 from 12 replicates - after the removal of 2 outlier samples using the Chauvenet criteria.

The pooled standard deviation was 0.0013 when using the complete set of 14 replicates.

### Duplicate samples from a single Niskin bottle

Event Number	Sample Number	Station	Pressure dbar	Salinity 1	Salinity 2	Rejected yes / no	Comment
18	154	P4	1249.9	34.4647	34.4601	yes	
18	155	P4	1001.1	34.3870	34.3829	yes	
26	253	P8	2000.0	34.5933	34.5932		
26	256	P8	1000.3	34.3799	34.3803		
31	291	P12	2500.0	34.6254	34.6250		
31	295	P12	1000.9	34.3571	34.3570		
45	431	P16	3001.2	34.6534	34.6531		
45	433	P16	2000.8	34.5889	34.5903		
45	436	P16	999.9	34.3733	34.3752		
53	483	P20	3000.2	34.6555	34.6562		
53	485	P20	2000.3	34.5845	34.5843		
53	488	P20	999.7	34.3639	34.3643		
72	601	P26	4000.8	34.6801	34.6813		
72	605	P26	1999.3	34.5789	34.5789		

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### Duplicate Niskins at the same pressure

Salinity: Bottle ranged from 34.4601 to 34.6711 with a standard deviation of 0.0006 ml/l from 4 replicates after the removal of 0 outlier sample using Chauvenet's criteria.

**Note:** Although the precision statement for samples drawn from duplicate Niskin bottles is calculated using the same formula as the precision statement for duplicate samples drawn from one single Niskin, this process is mainly used to identify problem samples and is not being used as a measure of analytical precision.

Event Number	Sample Number	Station	Nominal Pressure dbar	Salinity 1	Salinity 2	Rejected yes / no	Comment
18	153 / 154	P4	1250	34.4606	34.4601		
31	289 / 290	P12	3000	34.6476	34.6468		
45	429 / 430	P16	3500	34.6647	34.6661		
53	481 / 482	P20	3500	34.6709	34.6711		