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AIMS: Australia's tropical marine research agency

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Revision History

Version		Title	Name	Date	Comments
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4. EXPLORATORY DATA ANALYSIS

Exploratory data analysis is vital for informing data processing and analysis as well as establishing assumptions and limitations. Of particular importance for the current project is the spatial and temporal distribution and variability of the various data Measures and Sources. As such, a series of exploratory plots have been generated (see Appendix ?? beginning on page ??). In the interest of keeping the main text free of copious graphics, we have elected to present only a small fraction of the exploratory data analyses figures here. The figures presented will act as exemplars of general format and predominant features or patterns.

4.1 All data

Figures 1 – 4 display the temporal distribution of Chlorophyll-a, TSS, Secchi depth and NOx observations for the Wet Tropics Open Coastal Zone from AIMS insitu, AIMS FLNTU, Satellite, eReefs and eReefs926 sources.

All of the figures are presented with log-transformed y-axes as the data are typically positively skewed. This is expected for parameters that have a natural minimum (zero), yet no theoretical maximum. It does however mean that these distributional properties should be considered during the analyses. In particular, for mean based aggregations, outliers and skewed distributions can impart unrepresentative influence on outcomes.

Each of the data sources present different variability characteristics. The scale of the range of AIMS insitu data is predominantly and approximately less than or equal to the scale of the half/twice the associated threshold value (Fig. 1-4a). The AIMS FLNTU logger data (Fig. 1-4b) have a larger range than the AIMS insitu data - presumably because the former data collection frequency captures most of the peaks and trophs whereas the later are unlikely to do so. Furthermore, whilst the AIMS insitu data are predominantly collected during the dry season, the AIMS FLNTU loggers collect data across the entire year and are therefore likely to record a greater proportion of the full variation in conditions. Of course it is important when interpreting these diagnostic plots to focus mainly on the violin plots and less on the dots (representing individual observations). This is because the dots do not provide an indication of the density and it is easy to allow outliers to distort out impression of the variability of the data.

Similarly, the scale of the range eReefs and eReefs926 data (Fig. 1-4d-e) is approximately equal to the scale of the range of the span from half/twice the threshold value. This reflects both a more complete time series and broader spatial extent represented in the data. In contrast to the AIMS insitu and to a lesser extent the AIMS FLNTU and eReefs data, the scale of the range of the Satellite is relatively large - typically a greater span than the range of half/twice threshold value (Fig. 1-4c).

The Satellite, eReefs and eReefs926 data series all start and end part of the way through a water year. For annually aggregated data, this is likely to result in unrepresentative estimates and thus only full water years will be analysed.

4.2 Annual data

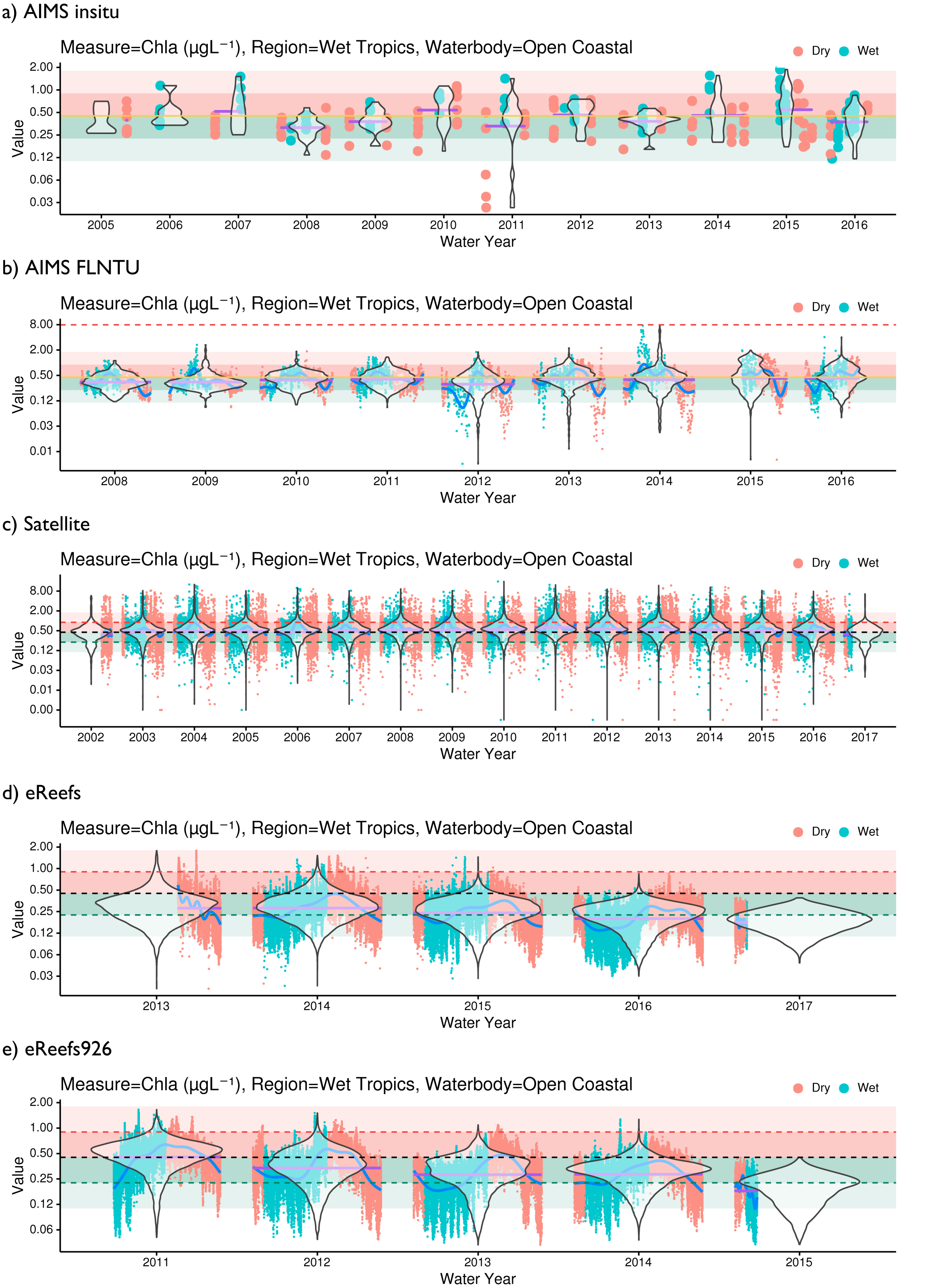


Figure 1: Observed (logarithmic axis with violin plot overlay) Chlorophyll-a data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) AIMS FLNTU, c) Satellite, d) eReefs and e) eReefs926. Observations are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Blue smoother represents Generalized Additive Mixed Model within a water year and purple line represents average within the water year. Horizontal red, black and green dashed lines denote the twice threshold, threshold and half threshold values respectively. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

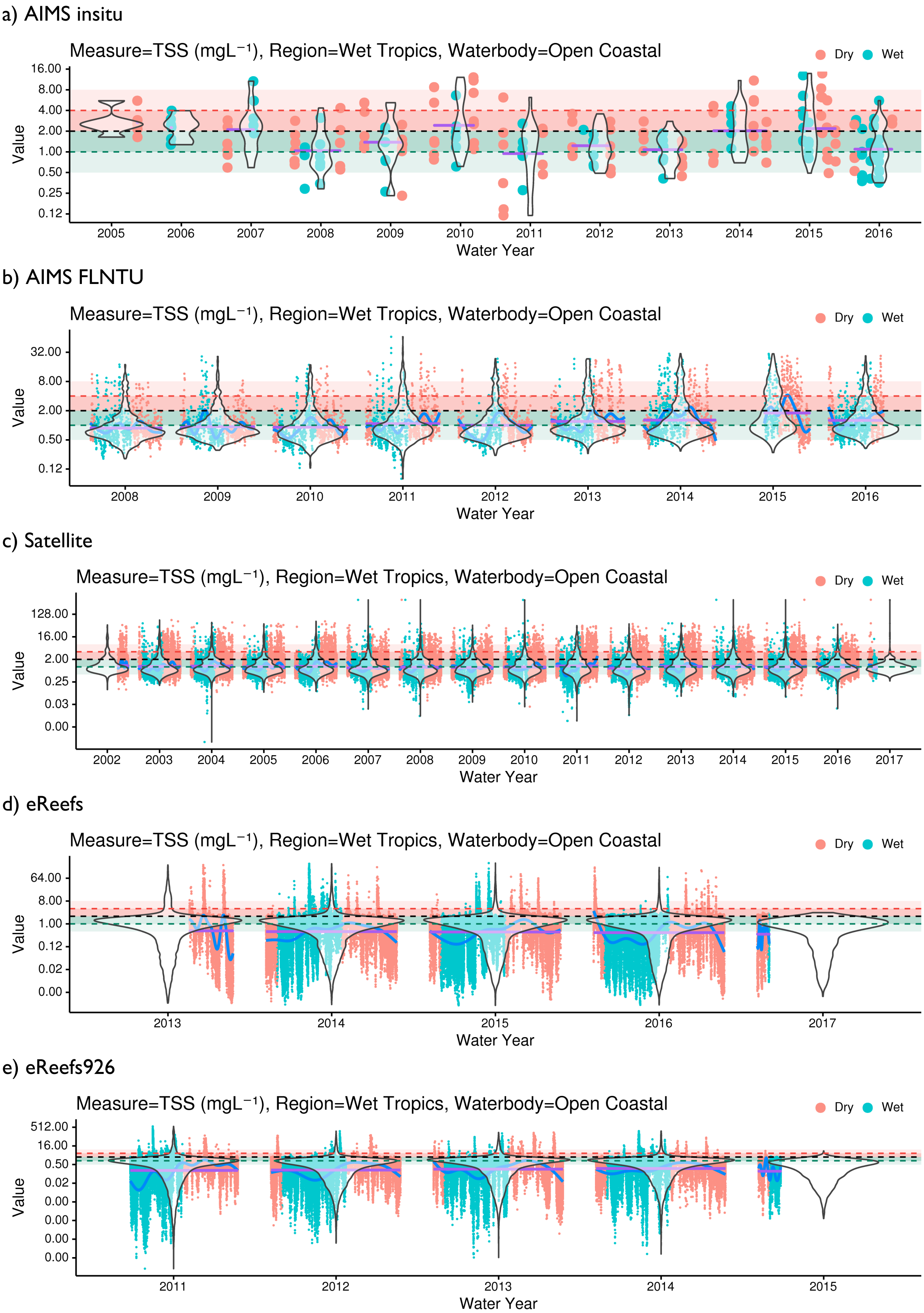


Figure 2: Observed (logarithmic axis with violin plot overlay) TSS data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) AIMS FLNTU, c) Satellite, d) eReefs and e) eReefs926. Observations are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Blue smoother represents Generalized Additive Mixed Model within a water year and purple line represents average within the water year. Horizontal red, black and green dashed lines denote the twice threshold, threshold and half threshold values respectively. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

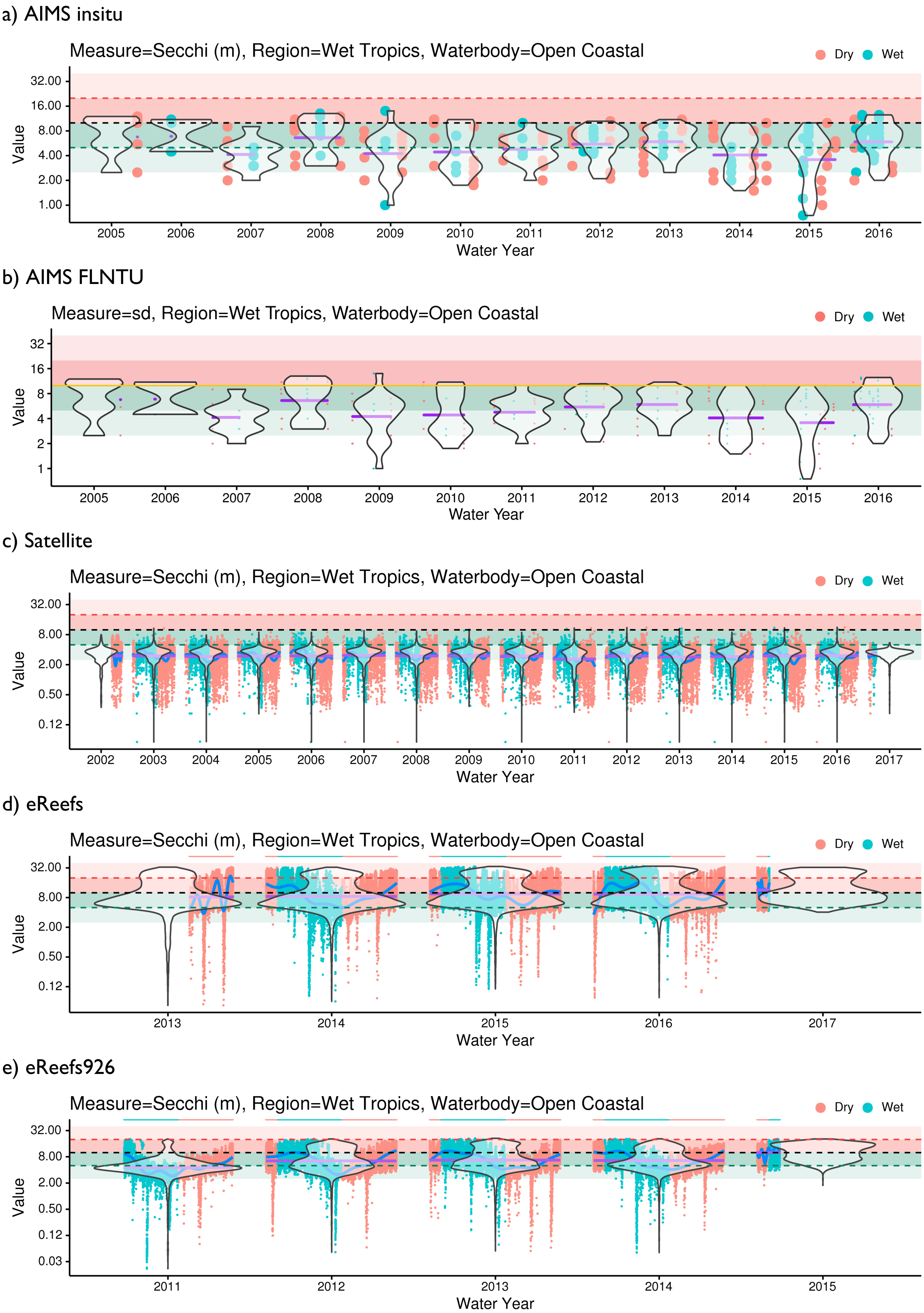
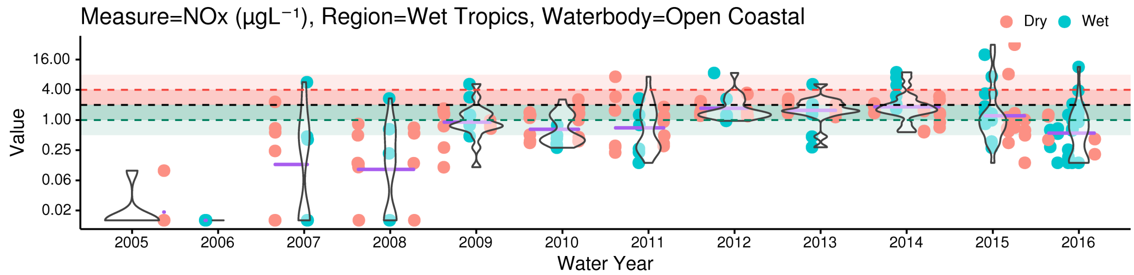
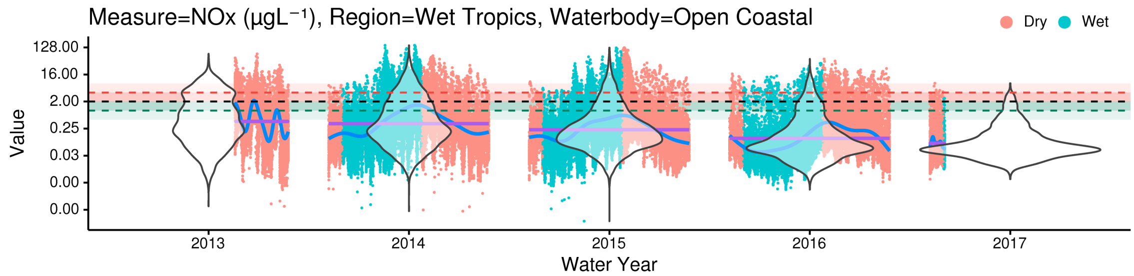


Figure 3: Observed (logarithmic axis with violin plot overlay) Secchi depth data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) AIMS FLNTU, c) Satellite, d) eReefs and e) eReefs926. Observations are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Blue smoother represents Generalized Additive Mixed Model within a water year and purple line represents average within the water year. Horizontal red, black and green dashed lines denote the twice threshold, threshold and half threshold values respectively. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

a) AIMS insitu



b) eReefs



c) eReefs926

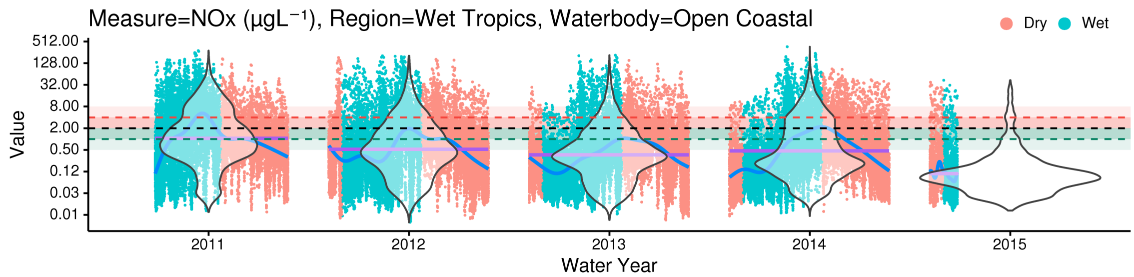


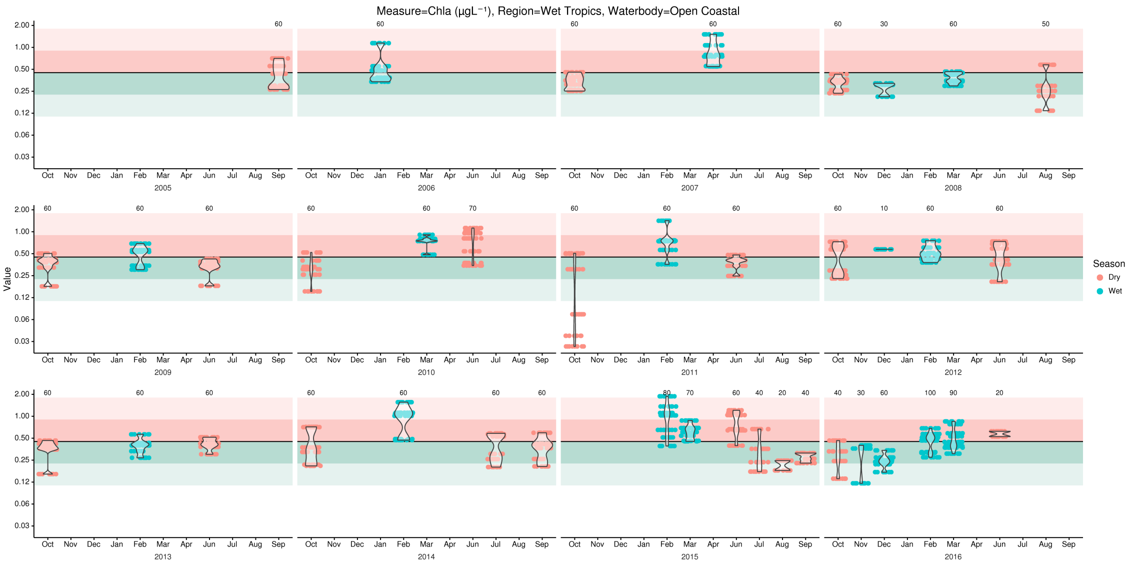
Figure 4: Observed (logarithmic axis with violin plot overlay) NOx data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) eReefs and c) eReefs926. Observations are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Blue smoother represents Generalized Additive Mixed Model within a water year and purple line represents average within the water year. Horizontal red, black and green dashed lines denote the twice threshold, threshold and half threshold values respectively. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

4.3 Monthly data

Figures 5 – 10 provide finer temporal resolution by displaying the temporal distribution of Chlorophyll-a, TSS, Secchi depth and NOx observations for the each month within Wet Tropics Open Coastal Zone from AIMS insitu, AIMS FLNTU, Satellite, eReefs and eReefs926 sources.

The monthly violin plots do not add any additional insights with respect to understanding the characteristics of the underlying data to help guide the selection of appropriate indexation formulation or perhaps even Measure/Source selection. Rather, they provide a less compacted view of the underlying data from which patterns highlighted in Section 4.2 might be more easily appreciated.

a) AIMS insitu



b) AIMS FLNTU

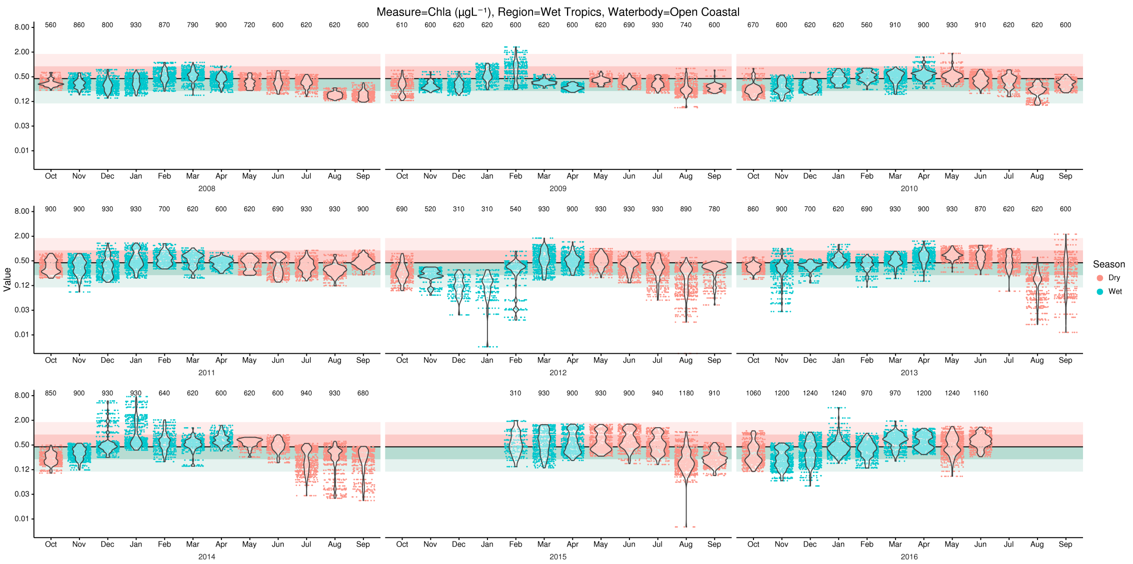
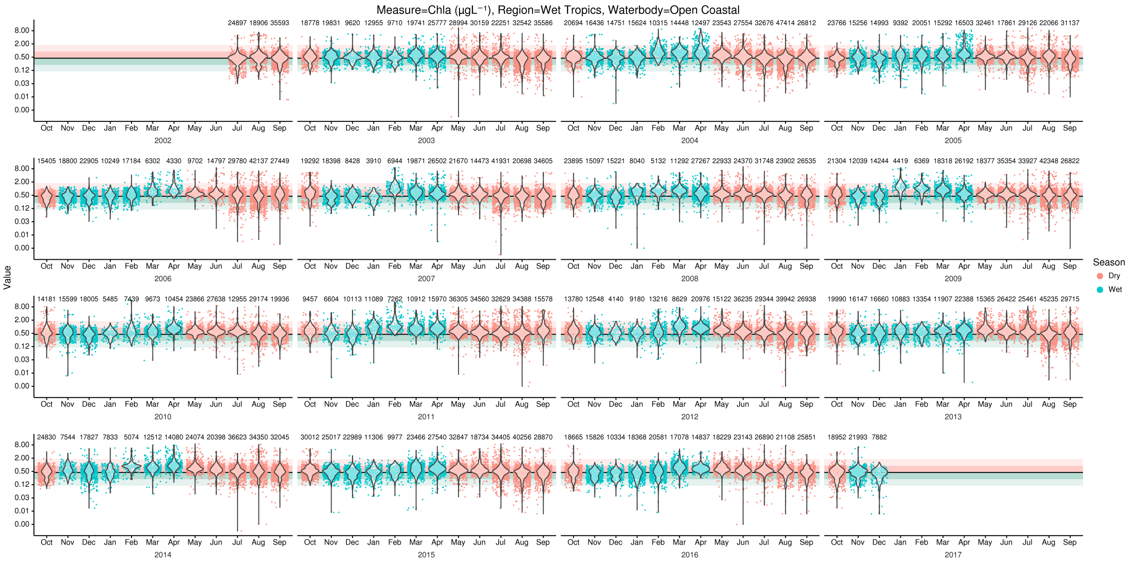


Figure 5: Observed (logarithmic axis with violin plot overlay) Chlorophyll-a data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) AIMS FLNTU. Observations grouped into months are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Sample sizes represented as numbers above violins and horizontal black dashed line denotes threshold value. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

a) Satellite



b) eReefs

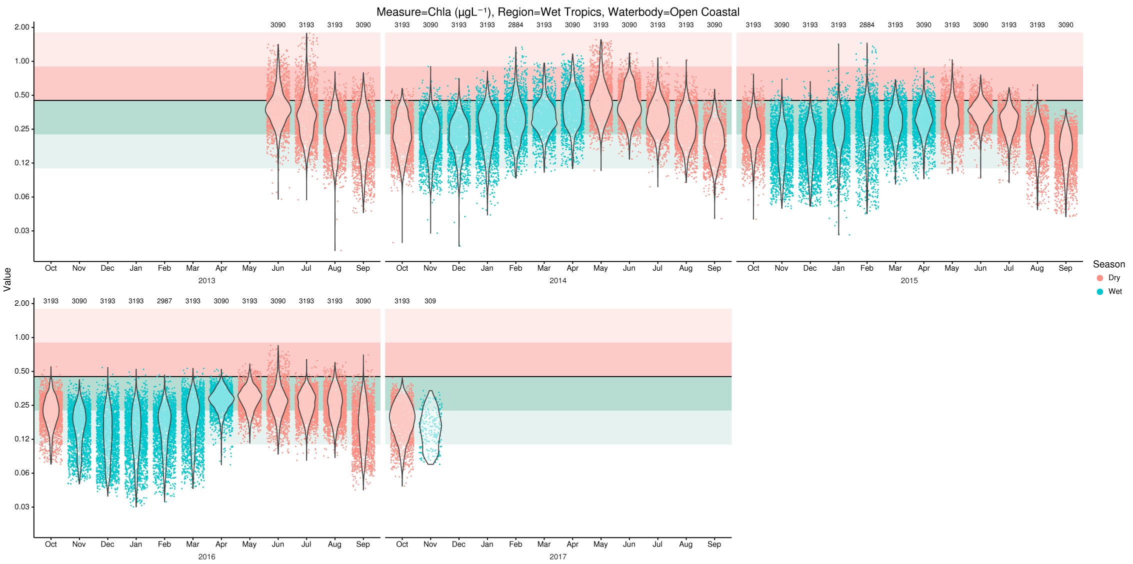
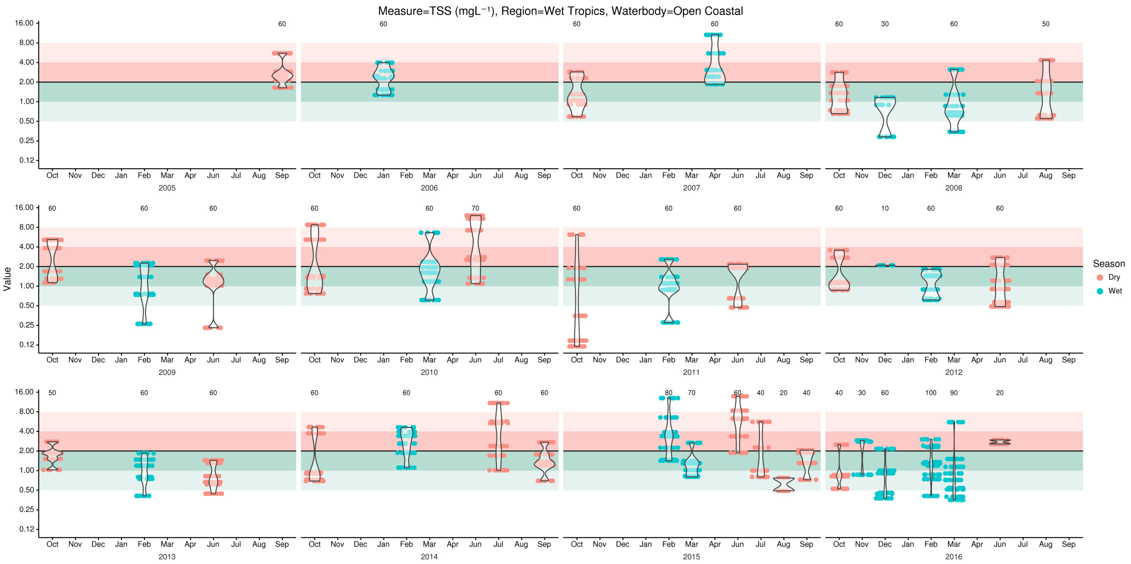


Figure 6: Observed (logarithmic axis with violin plot overlay) Chlorophyll-a data for the Wet Tropics Open Coastal Zone from a) Satellite, b) eReefs. Observations grouped into months are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Sample sizes represented as numbers above violins and horizontal black dashed line denotes threshold value. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

a) AIMS insitu



b) AIMS FLNTU

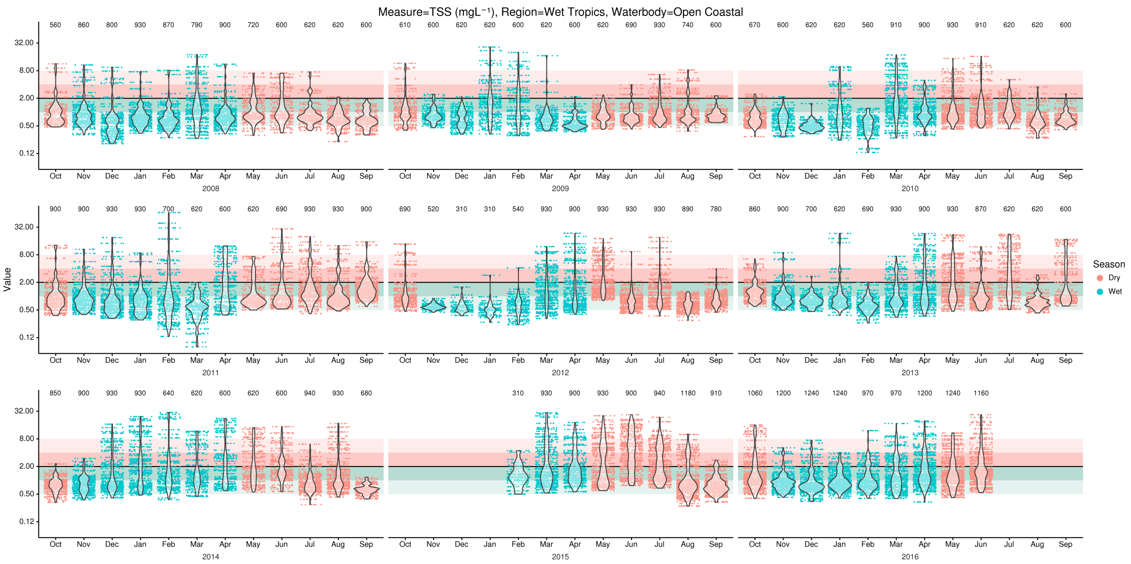
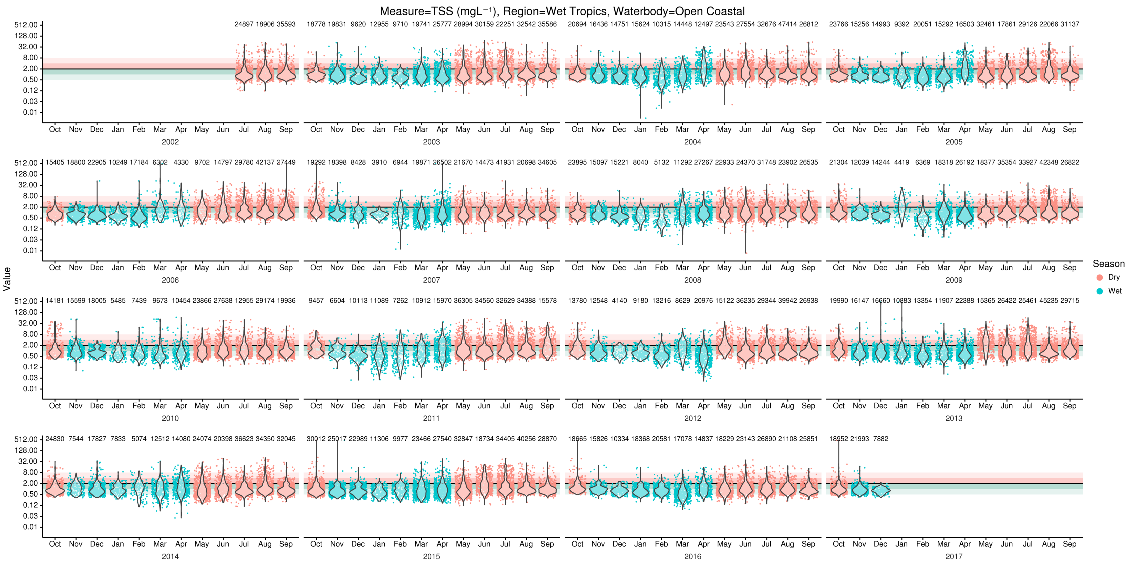


Figure 7: Observed (logarithmic axis with violin plot overlay) TSS data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) AIMS FLNTU. Observations grouped into months are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Sample sizes represented as numbers above violins and horizontal black dashed line denotes threshold value. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

a) Satellite



b) eReefs

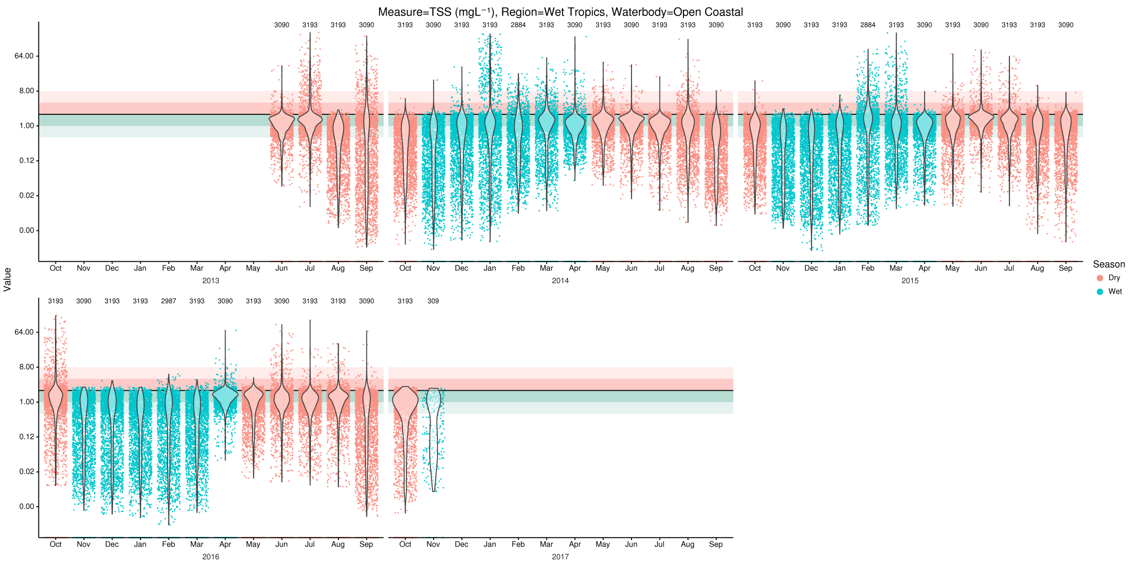
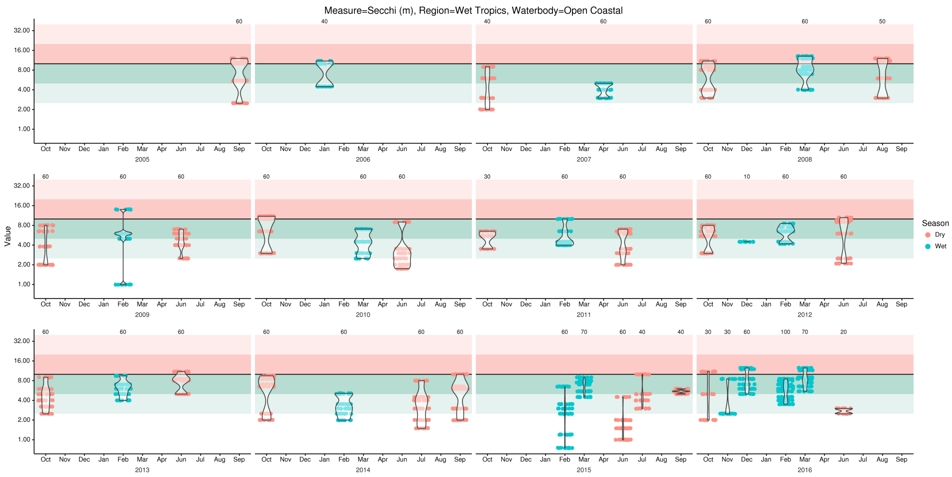
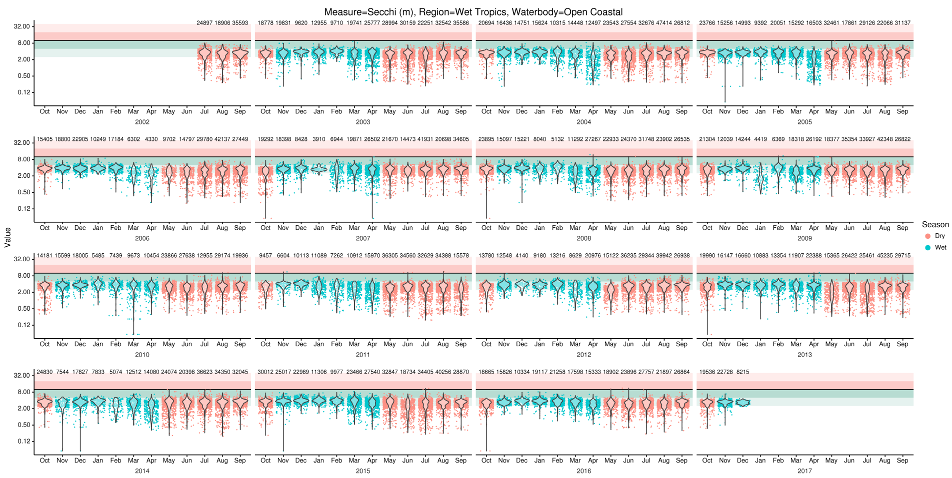


Figure 8: Observed (logarithmic axis with violin plot overlay) TSS data for the Wet Tropics Open Coastal Zone from a) Satellite, b) eReefs. Observations grouped into months are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Sample sizes represented as numbers above violins and horizontal black dashed line denotes threshold value. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

a) AIMS insitu



b) Satellite



c) eReefs

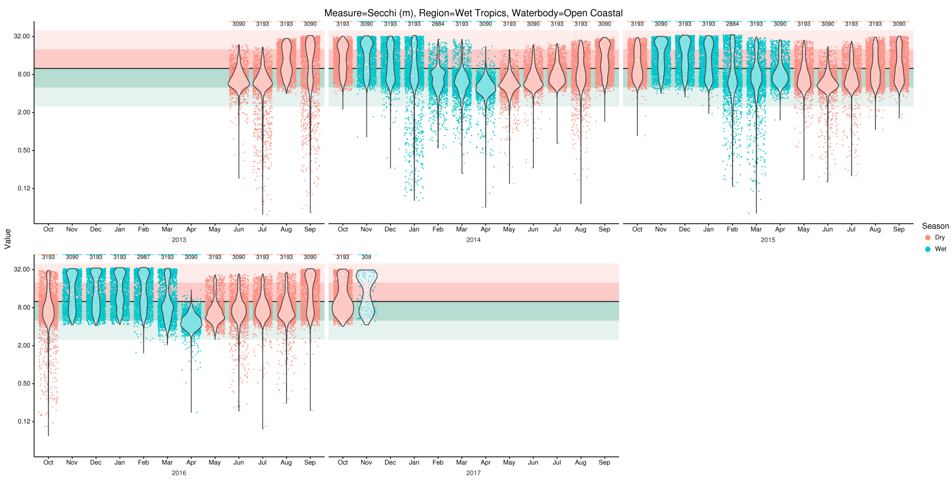
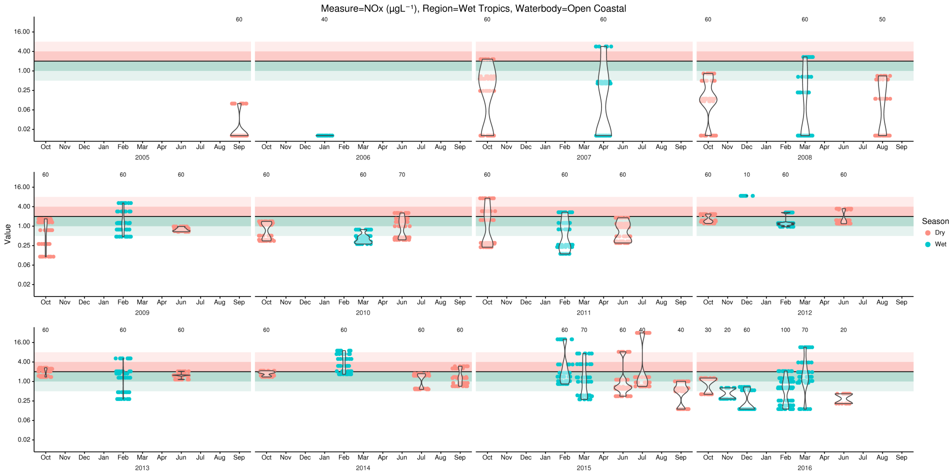
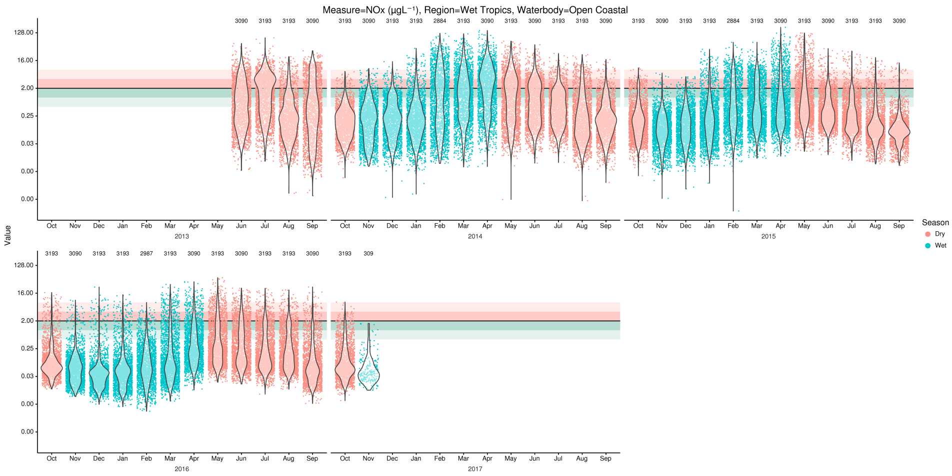


Figure 9: Observed (logarithmic axis with violin plot overlay) Secchi depth data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) Satellite and c) eReefs. Observations grouped into months are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Sample sizes represented as numbers above violins and horizontal black dashed line denotes threshold value. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

a) AIMS insitu



b) eReefs



c) eReefs926

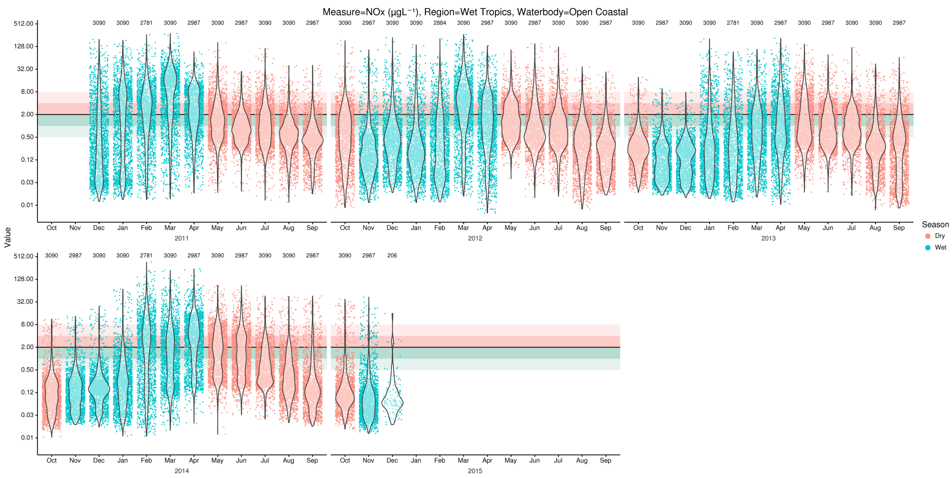


Figure 10: Observed (logarithmic axis with violin plot overlay) Secchi depth data for the Wet Tropics Open Coastal Zone from a) AIMS insitu, b) eReefs c) eReefs926. Observations grouped into months are ordered over time and colored conditional on season as Wet (blue symbols) and Dry (red symbols). Sample sizes represented as numbers above violins and horizontal black dashed line denotes threshold value. Red and green background shading indicates the range (10% shade: x4,/4; 30% shade: x2,/2) above and below threshold respectively.

4.4 Spatial data

Figures 11 – 18 explore the spatio-temporal patterns in observed data from a finer spatial perspective (again focussing on just the Wet Tropics Open Coastal and Dry Tropics Midshelf Zones). Importantly, the colour scales have been mapped to a constant value range for each source for a given Measure. The lower and upper bounds of the constant range is respectively based on twice and half the threshold (see Table ??) value (except for Secchi depth which are half and twice respectively). Half and double the threshold was considered broadly appropriate for the Insitu data and thus should also be broadly appropriate for the other sources since they are intended to be indirect approximations of direct sampling.

These figures also highlight the disparity in resolution between the different data sources. The AIMS insitu data is spatially very sparse [1]. The Satellite data has the most extensive spatial resolution and notwithstanding the many gaps due to various optical interferences (such as cloud cover), also has the greatest temporal coverage[2].

For the selected Zones and span of water years, there is little evidence of a major latitudinal gradient in Satellite Chlorophyll-a with most of any change (if any) occurring across the shelf. Indeed, Satellite parameters are relatively constant over space and time for the Dry Tropics Midshelf Zone (see Figs. 15–17b). Moreover, the spatial patterns of Satellite derived Chlorophyll-a and TSS appear relatively invariant between years (see Figs.11–17b).

The eReefs and eReefs926 do show some variability in spatial and temporal Chlorophyll-a and Secchi depth (see Figs. 11c-d,13c-d,15c-d and 17c-d), yet relatively little for TSS and NOx (at least for Dry Tropics Midshelf). Whilst this apparent lack of variability is largely an artefact of the colour scale mapping, the values of these Measures are constantly substantially below the threshold value and thus invariant on the scale considered appropriate for comparison against the associated thresholds..

[1] the AIMS FLNTU logger data is even more sparse and thus is not shown.

[2] The remote sensing Satellite data span a temporal range of 2002 through to 2017, although only the range 2010-2016 is displayed

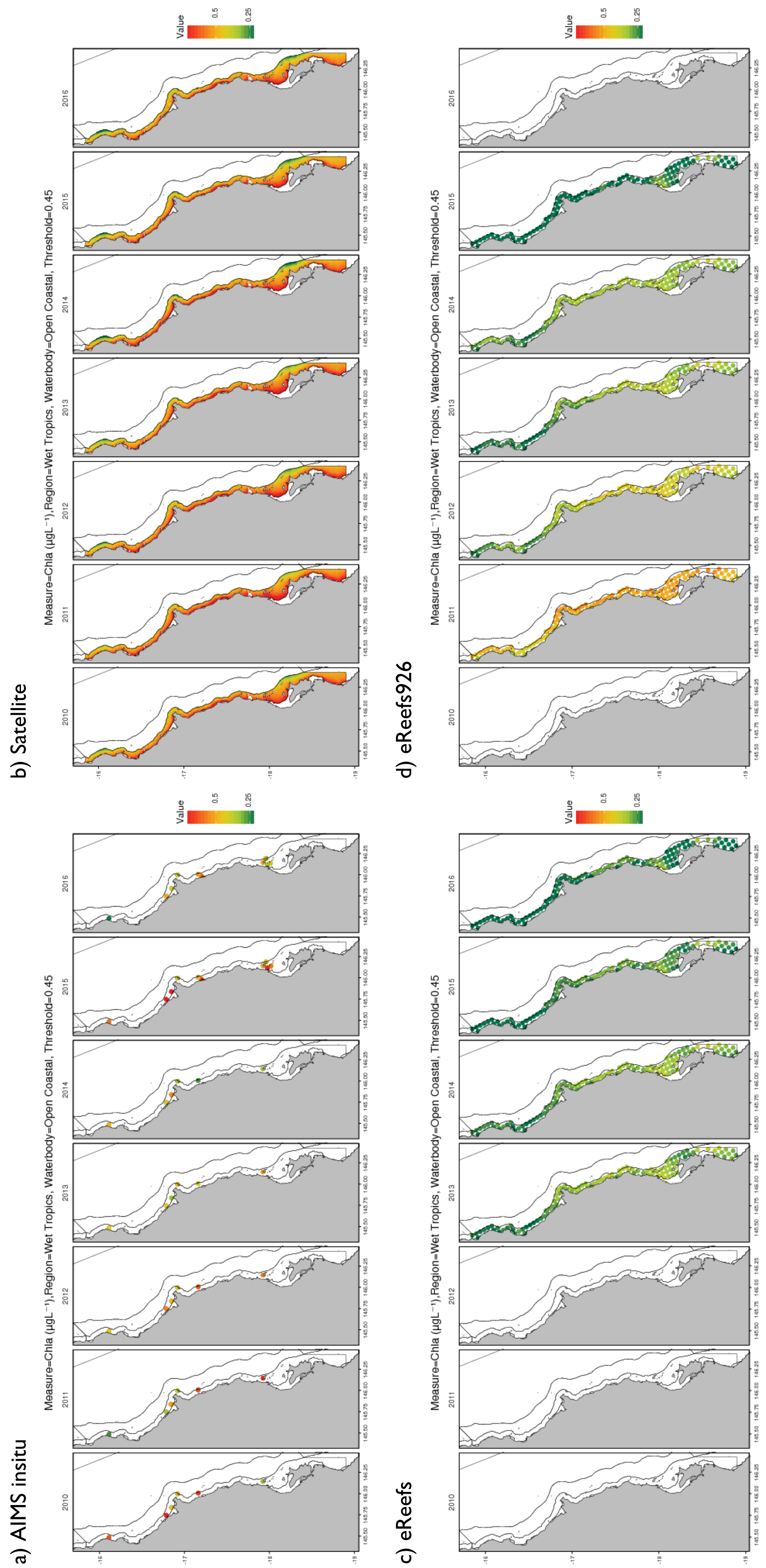


Figure 11: Spatial distribution of observed a) AIMS insitu, b) Satellite, c) eReefs and d) eReefs926 Chlorophyll-a (2009–2016) for the Wet Tropics Open Coastal Zone.

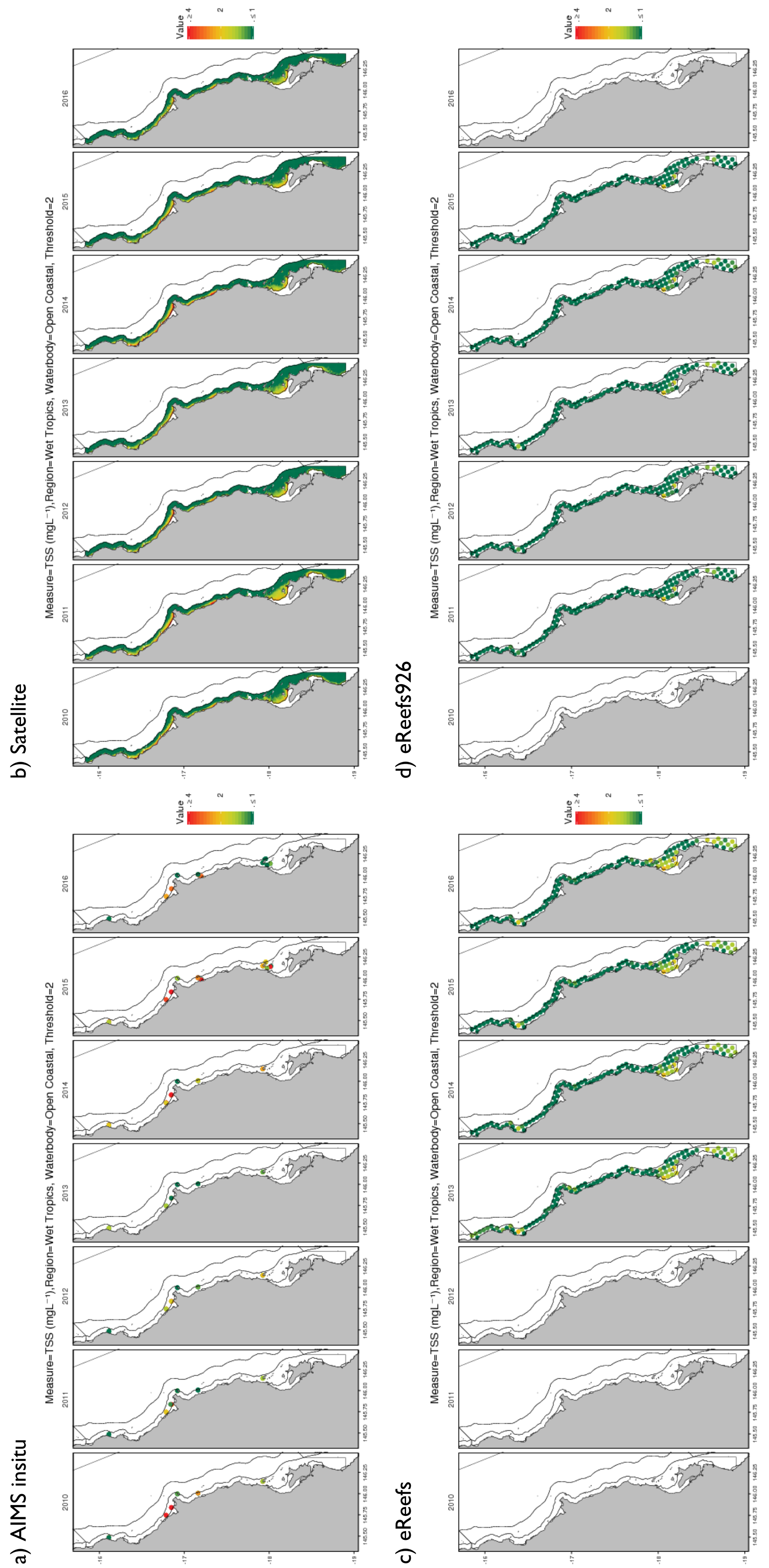


Figure 12: Spatial distribution of observed a) AIMS insitu, b) Satellite, c) eReefs and d) eReefs926 TSS (2009–2016) for the Wet Tropics Open Coastal Zone.

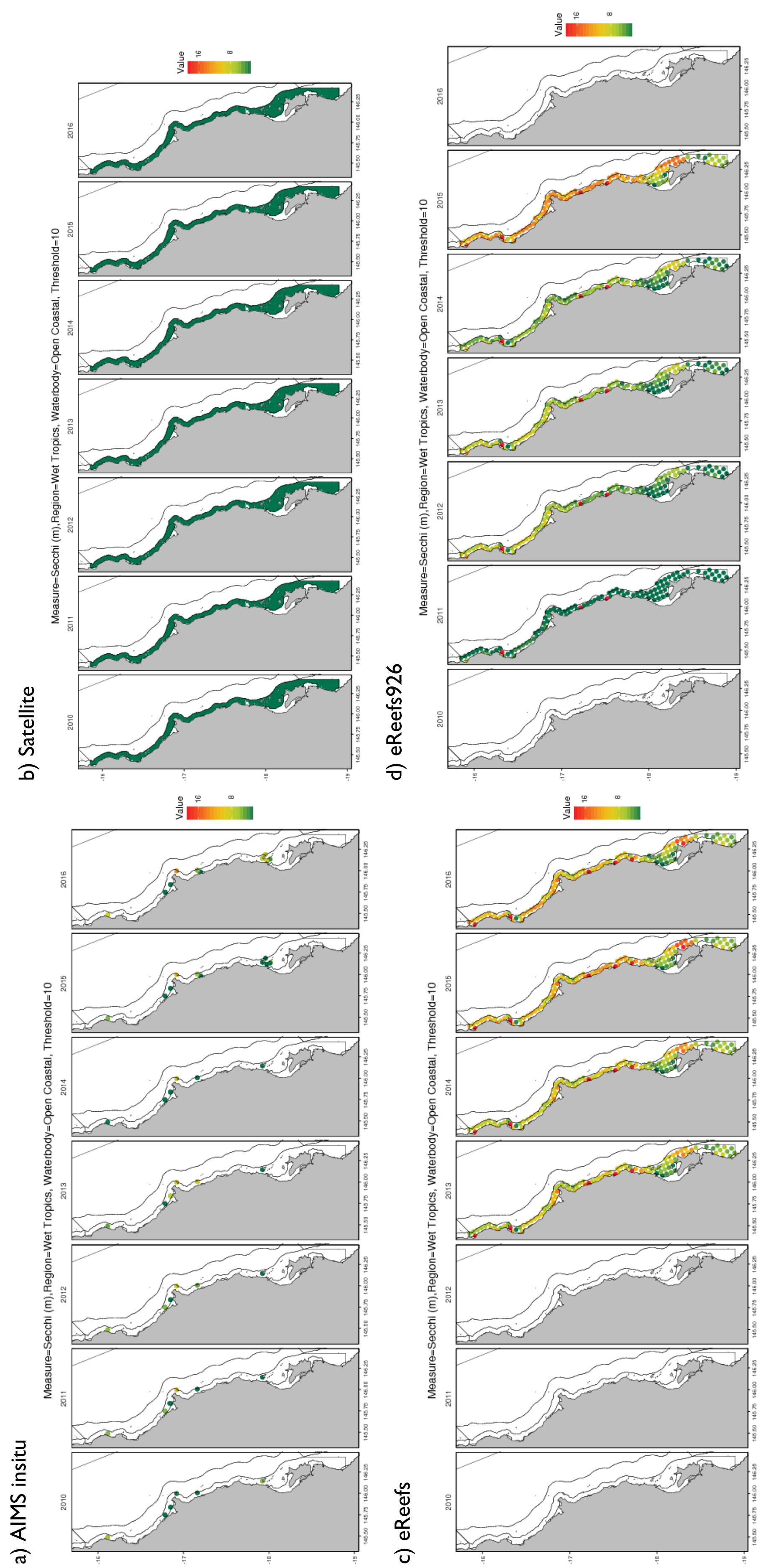


Figure 13: Spatial distribution of observed a) AIMS insitu, b) Satellite, c) eReefs and d) eReefs926 Secchi depth (2009–2016) for the Wet Tropics Open Coastal Zone.

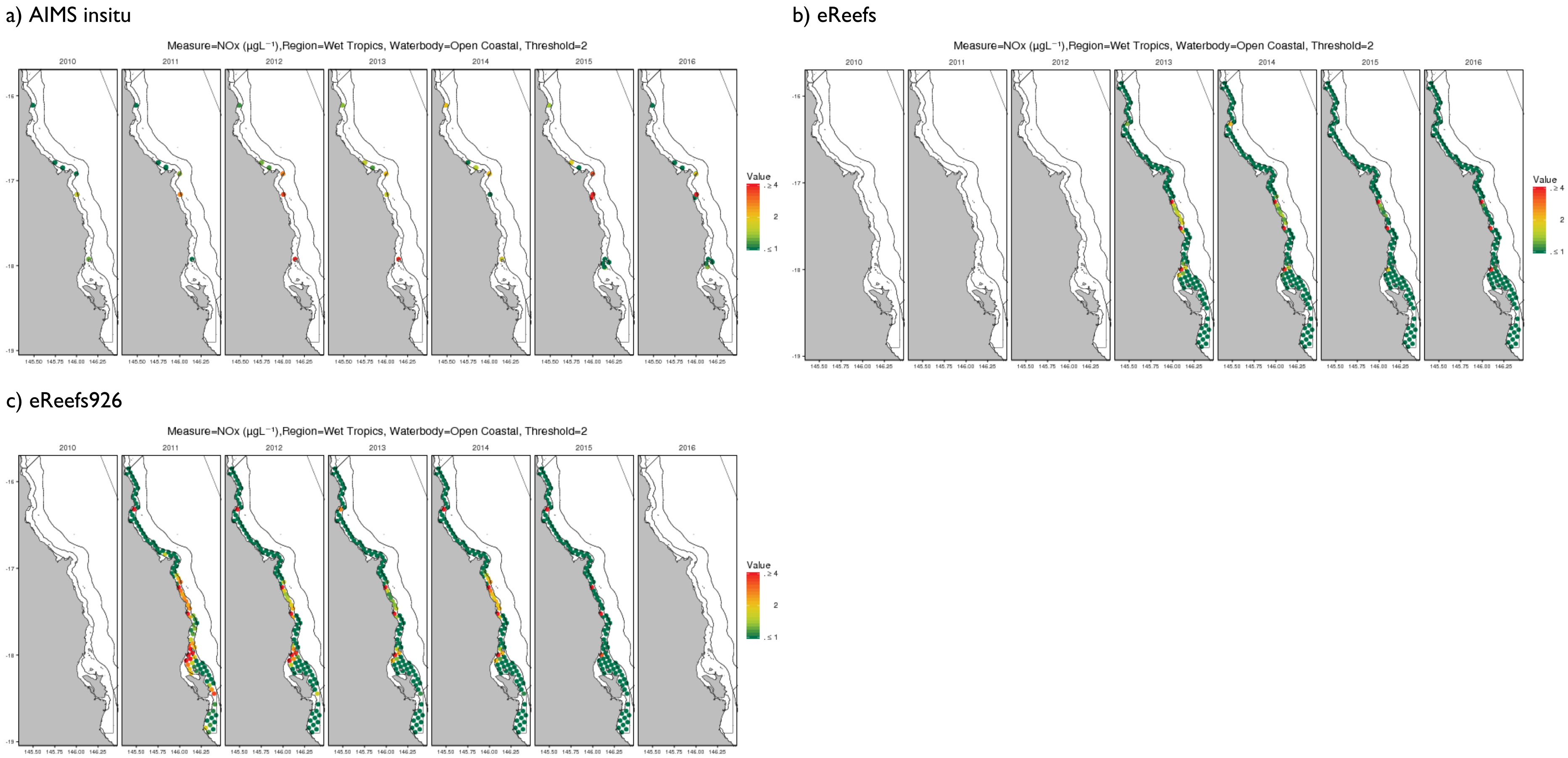


Figure 14: Spatial distribution of observed a) AIMS insitu, b) eReefs and c) eReefs926 NOx (2009–2016) for the Wet Tropics Open Coastal Zone.

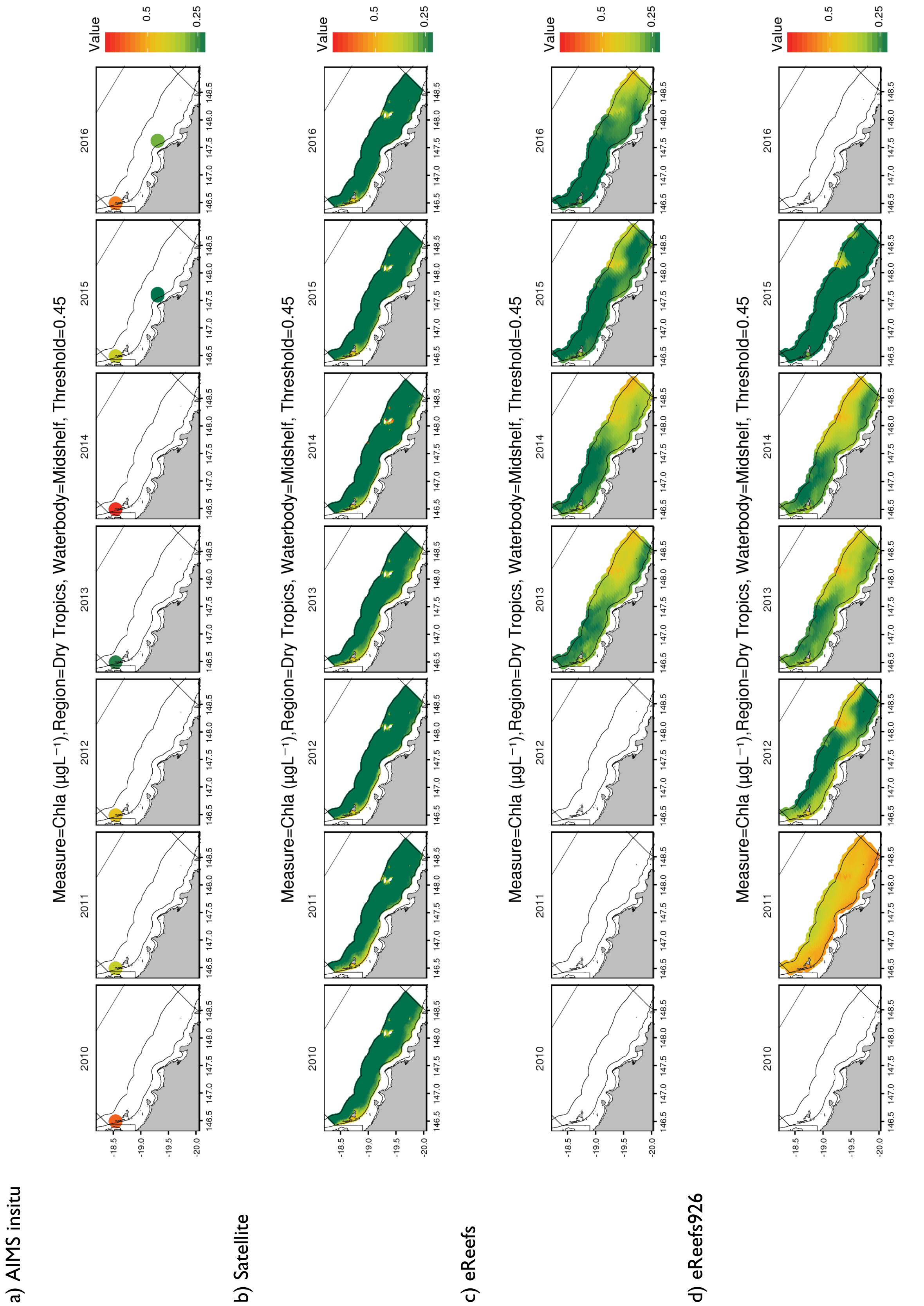


Figure 15: Spatial distribution of observed a) AIMS insitu, b) Satellite, c) eReefs and d) eReefs926 Chlorophyll-a (2009–2016) for the Dry Tropics Midshelf Zone.

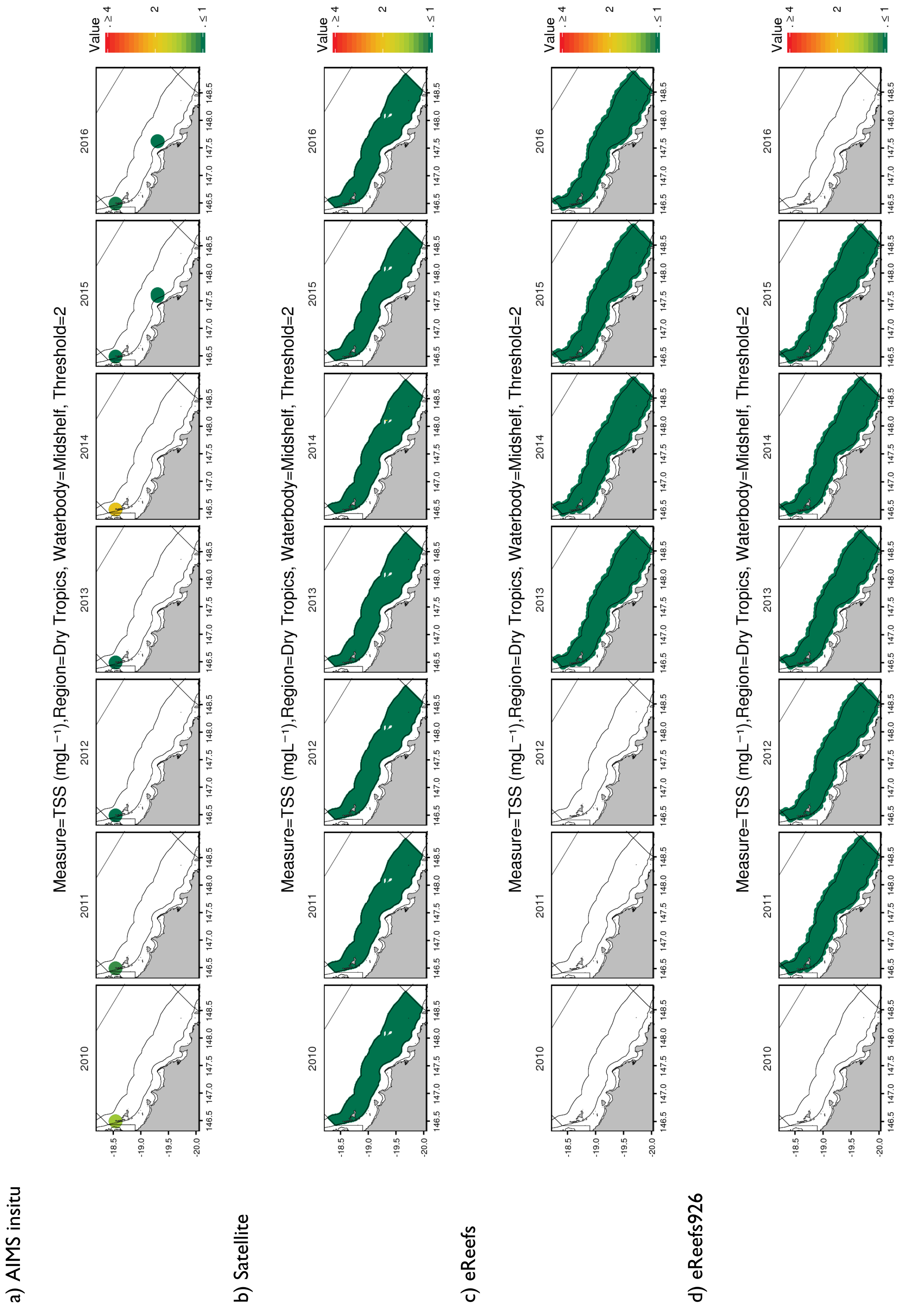


Figure 16: Spatial distribution of observed a) AIMS insitu, b) Satellite, c) eReefs and d) eReefs926 TSS (2009–2016) for the Dry Tropics Midshelf Zone.

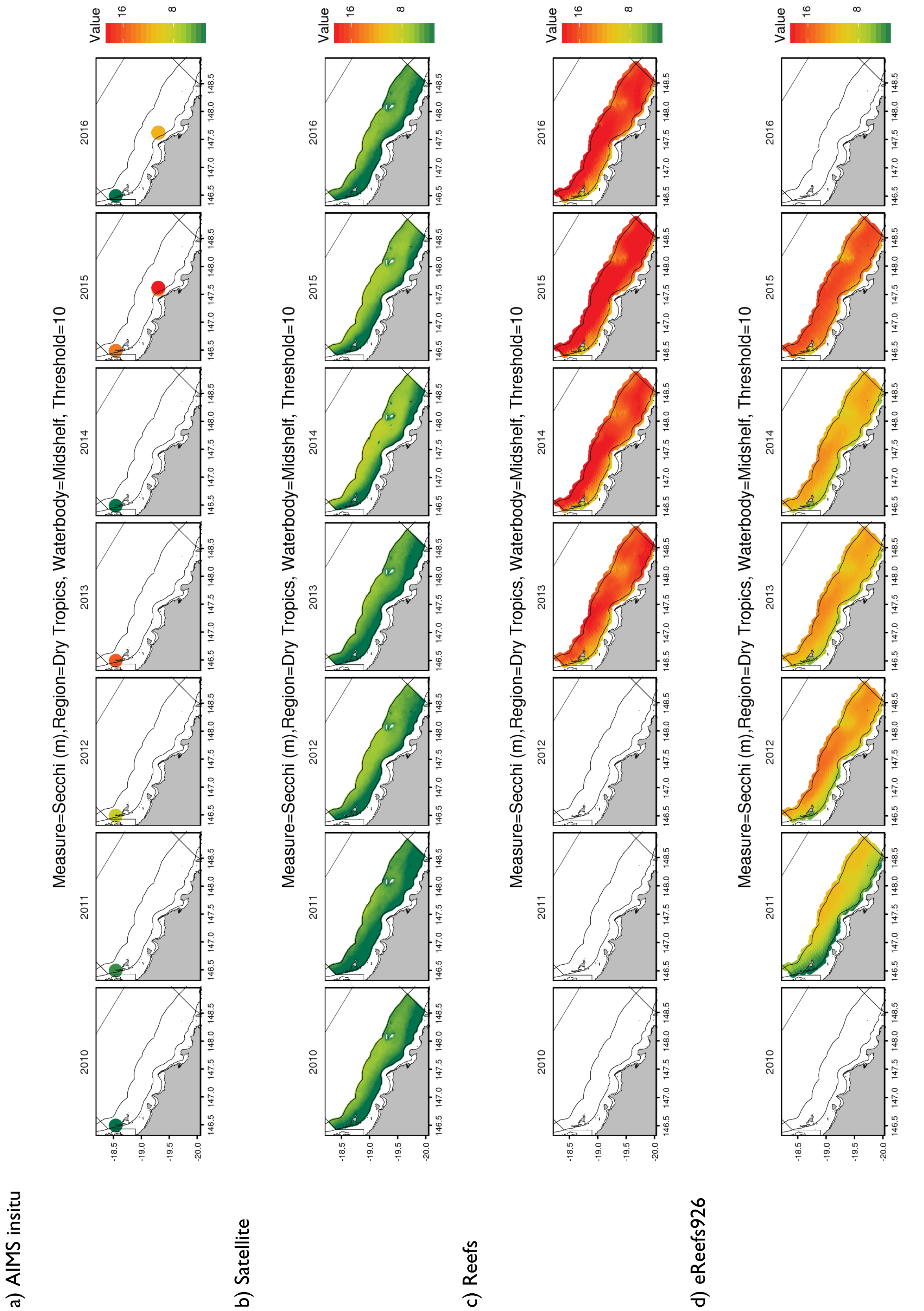
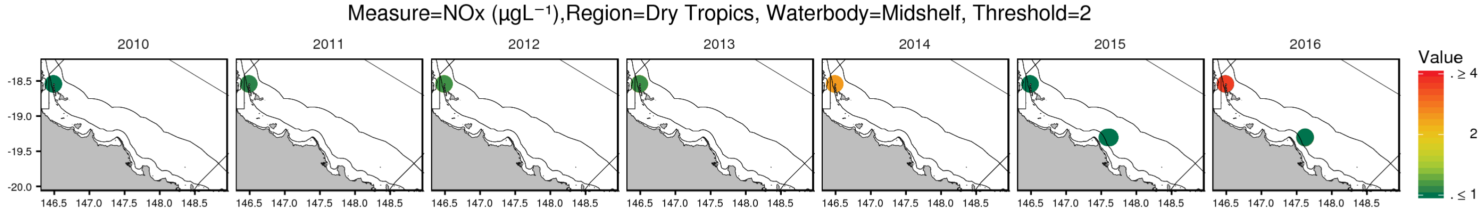
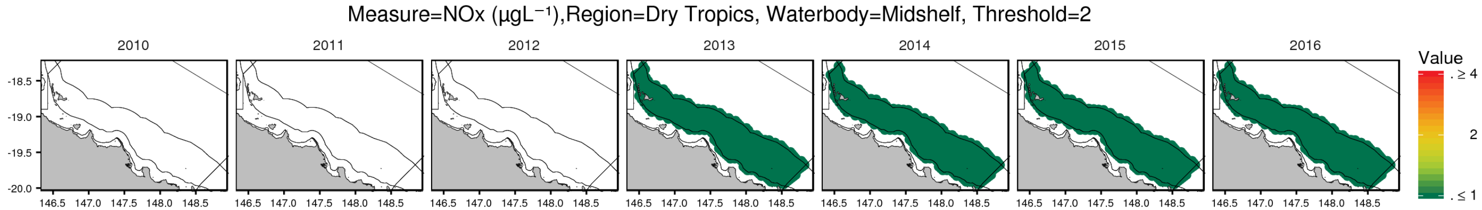


Figure 17: Spatial distribution of observed a) AIMS insitu, b) Satellite, c) eReefs and d) eReefs926 Secchi depth (2009–2016) for the Dry Tropics Midshelf Zone.

a) AIMS insitu



b) Reefs



c) eReefs926

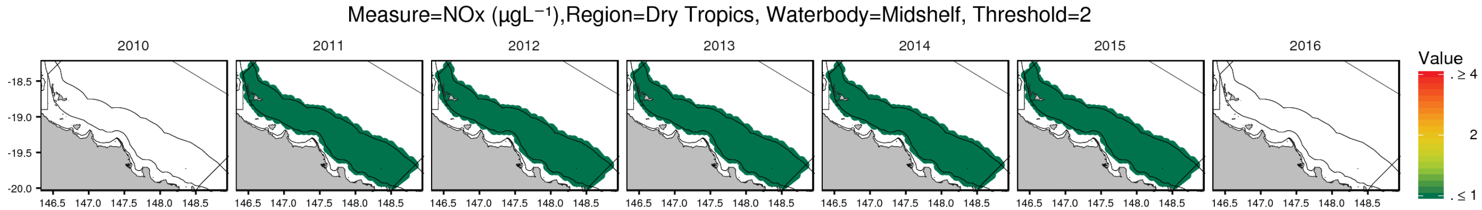


Figure 18: Spatial distribution of observed a) AIMS insitu, b) eReefs and c) eReefs926 NOx (2009–2016) for the Dry Tropics Midshelf Zone.

4.5 Comparison of data sources

Ensuring that the data underpinning the metric calculations are fit-for-purpose is a critical part of the process, especially if multiple data sources for a specific indicator are to be aggregated as part of these calculations. For example, successful aggregation of Chlorophyll-a as modelled by the eReefs BGC with Chlorophyll-a as extracted from satellite reflectance data (optical properties) will largely depend on the underlying compatibility of these two sources. Moreover, further combining with far more sparse and irregular sources (such as AIMS insitu Chlorophyll-a samples) relies on general patterns of spatial and temporal autocorrelation being present across the more dense data sources so as to facilitate a contagious projection of sparse data across the denser layers.

Based on substantial inconsistencies in the magnitude and variation of the observations between sources (AIMS insitu, Satellite and eReefs models), we recommend not to aggregating across the streams of data. Although it might be possible to normalize each source such that they do all have the same basic characteristics prior to aggregation[3], all the various approach to achieve normalization rely on the availability of independent estimates of either data reliability, accuracy or biases present in each source. Unfortunately, such information is not available.

Instead of aggregating the sources together, the preferred approach is to assimilate satellite reflectance information into the eReefs BGC model and to rely on in situ measurements for verification of the model performance.

It is worthwhile noting that there is no single point of truth as the sparse insitu sampling does not account for the dynamic nature of the receiving environment, both temporally and spatially. It is however possible to compare different measurement methods at a high level.

The five different sources (Satellite, eReefs, eReefs926, AIMS Insitu and AIMS FLNTU loggers) were all collected at different spatio-temporal resolutions. Specifically:

- the Satellite data are collected on a 1km grid on a daily basis, however there are many gaps in the time series of each cell due to cloud cover and other issues that affect the reliability of observations.
- the eReefs data are modelled and projected on to a 4km grid on a daily basis without any time series gaps between 2013 and 2016
- the eReefs926 data are modelled and projected on to a 4km grid on a daily basis without any time series gaps between 2011 and 2014
- the AIMS Insitu samples are collected from specific sampling sites (28-32 throughout the GBR) and on an infrequent basis (approx. 3-4 times per year although more frequently in later years). Furthermore, with the exception of relatively recently, the majority of samples were collected in the dry season and thus these samples could be biased towards long term water quality trends rather than short-term pulses.
- the AIMS FLNTU logger data are deployed at a subset (16) of the AIMS Insitu sampling locations and record measurements every 10 minutes (although there are frequent gaps due to instrument failure).

The AIMS Insitu sampling locations are strategically positioned so as to generally represent transects away from major rivers discharging into the GBR. As such, they likely represent biased estimates of the water parameters of the surrounding water bodies. Nevertheless, the observed data are direct measurements of a range of parameters considered to be important measures of water quality and are therefore considered to be relatively accurate estimates of the true state - albiet for a potentially narrow (and biased) spatio-temporal window. By contrast, the Satellite data represent indirect proxies for some of these parameters (Chlorophyll-a, Total Suspended Solids and Secchi Depth) and similarly, the eReefs data are indirect modelled estimates simulated from a deterministic manifestation of a conceptual model. Hence, to gauge the accuracy of the Satellite and eReefs data (and thus inform qualitative confidence), time series and spatial patterns in the Satellite and eReefs observations were compared to the AIMS Insitu observations.

The disparate spatio-temporal resolutions of the data sources present substantial challenges for extracting comparable data. For example, the proximity of AIMS Insitu samples to reefs and the spatial resolution (1km or 4km grid) frequently results in an inability to obtain matching spatial location for all three sources[4]. Furthermore, gaps in the Satellite time series frequently prevent matching Satellite data to the same day as AIMS Insitu sampling.

The degree to which the discrete AIMS Insitu samples reflect space and time around the actual sampling sites/times is largely unknown. That is, we don't know how broadly representative the direct observations are. Consequently,

[3] indeed this is one of the functions of indexing metrics (see section ??)

[4] Satellite data and eReefs models are of limited value in shallow water

it is difficult to estimate how broadly to filter the Satellite and eReefs data in space and time around the AIMS Insitu sampling events in order to generate comparable data. The 'best' breadth is likely to be a compromise between data availability (time limited for Satellite and space limited for eReefs).

Figures 19 and 20 illustrate the spatial distribution of Satellite and eReefs grid cell centroid locations relative to the AIMS Insitu sampling locations. The different color spokes denote distance categories (red: <1km, purple: <5km) from the AIMS Insitu data.

The approach we took was to extract all observations within a specific series of spatio-temporal windows or neighbourhoods from which we could calculate a range of association and correspondence (such as RMSE and R^2) metrics (see Tables 1, 2, 3 & 4). Tables 2, 3 & 4 document the top 5 ranked (according to RMSE, MAE and MAPE respectively) spatio-temporal lag associations between Satellite/eReefs data and AIMS Insitu data.

Table 1: Association and correspondence metrics between Satellite/eReefs observations ($\hat{\theta}_i$) and AIMS Niskin observations (θ_i). Similar calculations can be performed on model residuals.

Metric	Description	Formulation
RMSE	Root Mean Square Error - is a measure of accuracy	$RMSE(\hat{\theta}) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{\theta}_i - \theta_i)^2}$
MAE	Mean Absolute Error - is a measure of accuracy	$MAE(\hat{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\lvert(\hat{\theta}_i - \theta_i)\rvert$
MAPE	Mean Absolute Percentage Error - is a measure of accuracy expressed as a percentage of AIMS insitu samples	$MAPE(\hat{\theta}) = \frac{100}{n}\sum_{i=1}^{n}\frac{\hat{\theta}_i - \theta_i}{\theta_i}$

Whilst it is well established that water quality parameters can be highly varied over time and space, even approximate degrees of spatio-temporal autocorrelation for these parameters remains largely unknown. Nevertheless, we might expect that observations from different sources collected at similar locations and at similar times should be more similar to one another than they are to more distal observations. Furthermore, whilst the absolute values derived from different sources might not be exactly the same, we should expect a reasonable degree of correlation between the sources. Given these two positions (that observations should be autocorrelated and that different sources should be correlated), we should expect that the degree of correlation between the different sources for a given measure should be strongest for observation pairs closer together in space and time.

Tables 2 – 4 tabulate the association and correspondence metrics between the AIMS insitu samples and either the Satellite or eReefs data for each Measure. Irrespective of the association metric (RMSE, MAE or MAPE), closest associations with AIMS insitu observations tend to occur at shorter spatial distances for eReefs data than Satellite data, yet the opposite is apparent for temporal lags. We might have expected that associations would be strongest proximal (in both time and space) to the AIMS insitu samples and associations to weaken in some sort of multidimentional decaying pattern with increasing separation. Such a pattern would permit relatively straight forward integration of the AIMS insitu observational data into the Satellite or eReefs layers[5] However this is not the case and thus it is very difficult to formulate an integration routine that does more than just update a very limited number of points in space and time.

The other rationale for exploring the spatio-temporal associations between AIMS insitu data and Satellite/eReefs data is to be able to determine the optimal temporal lag and spatial distance for making comparisons of trends. Given that AIMS insitu data are in some respects considered the more accurate (albeit limited in the degree to which they more broadly represent space and time around the samples), a comparison of the general temporal trends of each source should give some idea of the relative accuracy of the sources of indirect measurements (Satellite and eReefs). Figures. 21 – 24 illustrate the temporal patterns of Chlorophyll-a, TSS, Secchi depth and NOx for each source (AIMS insitu, AIMS FLNTU, Satellite, eReefs and eReefs926) for each of the AIMS insitu sampling locations. The background fills of the site titles are colored according to water body (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

All sources of data are typically most variable at Enclosed Coastal sites and substantially less variable at Midshelf sites. Moreover, the alignment of trends also appears to be substantially better at Midshore sites. Enclosed

[5]Having a robust and consistent pattern of spatial and temporal autocorrelation would allow us to model the expected value of AIMS insitu data at unobserved locations.

Coastal and Open Coastal sites are closer to the coasts and in particular, closer to major sources of discharge (as intended by the AIMS Water Quality MMP) whereby water conditions are subject to more extreme fluctuations that result in conditions varying rapidly in time and space. Moreover, these sites are likely to be in shallower water or water whose depth is relatively heterogeneous. As a result, data pooled within a 5km radius might represent a substantially different body of water than that represented by the AIMS insitu point sources. By contrast, the conditions represented within a 5km radius at Midshelf sites are likely to be more homogeneous and thereby resulting in a fairer comparison.

Notwithstanding the disparity in fairness between different water bodies as a result of how well the various sources represent spatial and temporal envelopes, it is unlikely that either the eReefs models or Satellite data are going to provide accurate estimates for Enclosed Coastal water bodies. However, the accuracy for Midshelf and Offshore are likely to be sufficient.

Table 2: Top five ranked AIMS Niskin vs Satellite/eReefs observation association metrics (RMSE: root mean square error, MAE: mean absolute error, MAPE: mean percent error, Value: regression slope, residual.RMSE: residual root mean square error, residual.MAE: residual mean absolute error, R2.marginal: R^2 marginalized over sites, R2.conditional: R^2 conditional on sites) per Measure per source (Satellite, eReefs) for spatial/temporal lags. Rows ranked and filtered based on RMSE. Dist and Lag represent spatial (km) and temporal (days) lags.

Source	Measure	Dist	Lag	RMSE	MAE	MAPE	Value	Std.Error	DF	t.value	p.value	residual.RMSE	residual.MAE	R2.marginal	R2.conditional
Satellite	chl	8.00	6.00	0.33	0.22	0.69	0.42	0.04	566.00	11.43	0.00	0.22	0.14	0.10	0.66
Satellite	chl	9.00	6.00	0.33	0.22	0.69	0.42	0.04	566.00	11.37	0.00	0.22	0.14	0.09	0.67
Satellite	chl	6.00	6.00	0.33	0.22	0.69	0.43	0.04	566.00	11.54	0.00	0.22	0.14	0.10	0.65
Satellite	chl	10.00	6.00	0.33	0.22	0.69	0.42	0.04	566.00	11.30	0.00	0.22	0.13	0.09	0.67
Satellite	chl	11.00	6.00	0.33	0.22	0.69	0.42	0.04	566.00	11.27	0.00	0.22	0.13	0.09	0.67
eReefs	chl	1.00	5.00	0.34	0.24	0.44	0.13	0.03	96.00	3.67	0.00	0.10	0.08	0.08	0.48
eReefs	chl	1.00	4.00	0.34	0.24	0.44	0.14	0.04	96.00	3.85	0.00	0.10	0.08	0.09	0.48
eReefs	chl	1.00	6.00	0.34	0.24	0.45	0.12	0.03	96.00	3.63	0.00	0.09	0.08	0.08	0.49
eReefs	chl	1.00	3.00	0.34	0.24	0.45	0.16	0.04	96.00	3.76	0.00	0.12	0.09	0.09	0.42
eReefs	chl	1.00	7.00	0.34	0.24	0.45	0.11	0.03	96.00	3.46	0.00	0.09	0.07	0.07	0.50
Satellite	nap	4.00	1.00	1.65	0.90	1.02	0.48	0.03	432.00	16.60	0.00	1.15	0.54	0.40	0.45
Satellite	nap	1.00	1.00	1.66	0.87	1.08	0.54	0.04	358.00	14.58	0.00	1.30	0.57	0.38	0.45
Satellite	nap	4.00	0.00	1.67	0.87	1.21	0.51	0.04	225.00	13.99	0.00	1.17	0.52	0.45	0.49
Satellite	nap	3.00	1.00	1.70	0.91	0.97	0.47	0.03	427.00	15.41	0.00	1.19	0.55	0.37	0.43
Satellite	nap	3.00	0.00	1.73	0.90	1.11	0.54	0.04	214.00	13.28	0.00	1.23	0.57	0.43	0.53
eReefs	nap	5.00	3.00	2.07	1.18	0.73	0.12	0.02	239.00	6.20	0.00	0.57	0.38	0.13	0.16
eReefs	nap	5.00	4.00	2.07	1.17	0.73	0.11	0.02	239.00	5.51	0.00	0.56	0.39	0.11	0.16
eReefs	nap	4.00	3.00	2.08	1.17	0.70	0.11	0.02	239.00	5.78	0.00	0.53	0.37	0.12	0.18
eReefs	nap	4.00	4.00	2.08	1.16	0.70	0.09	0.02	239.00	5.03	0.00	0.54	0.39	0.09	0.16
eReefs	nap	5.00	2.00	2.08	1.18	0.74	0.12	0.02	239.00	6.00	0.00	0.57	0.39	0.13	0.16
Satellite	sd	5.00	2.00	4.47	3.38	0.44	0.11	0.01	463.00	11.77	0.00	0.55	0.42	0.24	0.54
Satellite	sd	4.00	2.00	4.48	3.38	0.44	0.11	0.01	462.00	11.71	0.00	0.56	0.42	0.24	0.52
Satellite	sd	3.00	2.00	4.48	3.39	0.44	0.12	0.01	455.00	11.73	0.00	0.57	0.42	0.25	0.51
Satellite	sd	11.00	2.00	4.48	3.37	0.44	0.11	0.01	470.00	11.65	0.00	0.53	0.41	0.20	0.61
Satellite	sd	12.00	2.00	4.48	3.37	0.44	0.11	0.01	470.00	11.65	0.00	0.53	0.41	0.20	0.61
eReefs	sd	4.00	1.00	13.13	11.31	2.37	1.23	0.12	196.00	10.39	0.00	6.47	4.92	0.35	0.37
eReefs	sd	4.00	2.00	13.29	11.68	2.49	1.14	0.11	196.00	9.89	0.00	6.10	4.75	0.34	0.37
eReefs	sd	5.00	1.00	13.46	11.62	2.36	1.29	0.12	185.00	10.81	0.00	6.61	5.12	0.38	0.39
eReefs	sd	6.00	1.00	13.53	11.69	2.37	1.30	0.13	185.00	10.40	0.00	6.43	4.96	0.38	0.41
eReefs	sd	5.00	2.00	13.66	12.02	2.48	1.18	0.12	185.00	10.20	0.00	6.30	5.02	0.36	0.37

Table 3: Top five ranked AIMS Niskin vs Satellite/eReefs observation association metrics (RMSE: root mean square error, MAE: mean absolute error, MAPE: mean percent error, Value: regression slope, residual.RMSE: residual root mean square error, residual.MAE: residual mean absolute error, R2.marginal: R^2 marginalized over sites, R2.conditional: R^2 conditional on sites) per Measure per source (Satellite, eReefs) for spatial/temporal lags. Rows ranked and filtered based on MAE. Dist and Lag represent spatial (km) and temporal (days) lags.

Source	Measure	Dist	Lag	RMSE	MAE	MAPE	Value	Std.Error	DF	t.value	p.value	residual.RMSE	residual.MAE	R2.marginal	R2.conditional
Satellite	chl	10.00	0.00	0.38	0.21	0.64	0.82	0.08	253.00	9.99	0.00	0.33	0.17	0.27	0.37
Satellite	chl	11.00	0.00	0.38	0.21	0.65	0.81	0.08	254.00	9.89	0.00	0.33	0.17	0.26	0.38
Satellite	chl	12.00	0.00	0.38	0.21	0.65	0.81	0.08	254.00	9.89	0.00	0.33	0.17	0.26	0.38
Satellite	chl	4.00	0.00	0.38	0.21	0.65	0.91	0.08	226.00	10.82	0.00	0.33	0.17	0.32	0.44
Satellite	chl	9.00	0.00	0.39	0.21	0.64	0.84	0.09	250.00	9.86	0.00	0.35	0.17	0.27	0.36
eReefs	chl	3.00	5.00	0.34	0.23	0.43	0.14	0.02	221.00	6.09	0.00	0.09	0.08	0.11	0.46
eReefs	chl	3.00	6.00	0.34	0.23	0.43	0.13	0.02	221.00	6.09	0.00	0.09	0.07	0.11	0.46
eReefs	chl	3.00	4.00	0.34	0.23	0.43	0.14	0.02	221.00	6.09	0.00	0.10	0.08	0.11	0.45
eReefs	chl	3.00	7.00	0.35	0.23	0.43	0.12	0.02	221.00	5.88	0.00	0.09	0.07	0.10	0.46
eReefs	chl	4.00	5.00	0.34	0.23	0.43	0.13	0.02	239.00	5.98	0.00	0.09	0.07	0.10	0.46
Satellite	nap	4.00	0.00	1.67	0.87	1.21	0.51	0.04	225.00	13.99	0.00	1.17	0.52	0.45	0.49
Satellite	nap	1.00	1.00	1.66	0.87	1.08	0.54	0.04	358.00	14.58	0.00	1.30	0.57	0.38	0.45
Satellite	nap	4.00	1.00	1.65	0.90	1.02	0.48	0.03	432.00	16.60	0.00	1.15	0.54	0.40	0.45
Satellite	nap	3.00	0.00	1.73	0.90	1.11	0.54	0.04	214.00	13.28	0.00	1.23	0.57	0.43	0.53
Satellite	nap	3.00	1.00	1.70	0.91	0.97	0.47	0.03	427.00	15.41	0.00	1.19	0.55	0.37	0.43
eReefs	nap	4.00	4.00	2.08	1.16	0.70	0.09	0.02	239.00	5.03	0.00	0.54	0.39	0.09	0.16
eReefs	nap	4.00	3.00	2.08	1.17	0.70	0.11	0.02	239.00	5.78	0.00	0.53	0.37	0.12	0.18
eReefs	nap	4.00	2.00	2.09	1.17	0.72	0.11	0.02	239.00	5.52	0.00	0.55	0.38	0.11	0.18
eReefs	nap	5.00	4.00	2.07	1.17	0.73	0.11	0.02	239.00	5.51	0.00	0.56	0.39	0.11	0.16
eReefs	nap	5.00	3.00	2.07	1.18	0.73	0.12	0.02	239.00	6.20	0.00	0.57	0.38	0.13	0.16
Satellite	sd	11.00	2.00	4.48	3.37	0.44	0.11	0.01	470.00	11.65	0.00	0.53	0.41	0.20	0.61
Satellite	sd	12.00	2.00	4.48	3.37	0.44	0.11	0.01	470.00	11.65	0.00	0.53	0.41	0.20	0.61
Satellite	sd	10.00	2.00	4.48	3.37	0.44	0.11	0.01	470.00	11.67	0.00	0.53	0.41	0.20	0.61
Satellite	sd	4.00	2.00	4.48	3.38	0.44	0.11	0.01	462.00	11.71	0.00	0.56	0.42	0.24	0.52
Satellite	sd	9.00	2.00	4.49	3.38	0.44	0.11	0.01	468.00	11.89	0.00	0.53	0.41	0.22	0.60
eReefs	sd	4.00	1.00	13.13	11.31	2.37	1.23	0.12	196.00	10.39	0.00	6.47	4.92	0.35	0.37
eReefs	sd	1.00	1.00	14.04	11.52	2.73	1.10	0.29	85.00	3.86	0.00	7.61	5.43	0.15	0.22
eReefs	sd	1.00	2.00	13.71	11.58	2.79	1.12	0.26	85.00	4.31	0.00	6.87	5.36	0.18	0.26
eReefs	sd	5.00	1.00	13.46	11.62	2.36	1.29	0.12	185.00	10.81	0.00	6.61	5.12	0.38	0.39
eReefs	sd	4.00	2.00	13.29	11.68	2.49	1.14	0.11	196.00	9.89	0.00	6.10	4.75	0.34	0.37

Table 4: Top five ranked AIMS Niskin vs Satellite/eReefs observation association metrics (RMSE: root mean square error, MAE: mean absolute error, MAPE: mean percent error, Value: regression slope, residual.RMSE: residual root mean square error, residual.MAE: residual mean absolute error, R2.marginal: R^2 marginalized over sites, R2.conditional: R^2 conditional on sites) per Measure per source (Satellite, eReefs) for spatial/temporal lags. Rows ranked and filtered based on MAPE. Dist and Lag represent spatial (km) and temporal (days) lags.

Source	Measure	Dist	Lag	RMSE	MAE	MAPE	Value	Std.Error	DF	t.value	p.value	residual.RMSE	residual.MAE	R2.marginal	R2.conditional
Satellite	chl	4.00	2.00	0.37	0.21	0.62	0.64	0.05	508.00	12.12	0.00	0.30	0.15	0.18	0.48
Satellite	chl	3.00	2.00	0.37	0.21	0.63	0.67	0.05	501.00	12.20	0.00	0.30	0.15	0.19	0.46
Satellite	chl	2.00	2.00	0.35	0.21	0.63	0.63	0.05	492.00	12.64	0.00	0.27	0.15	0.19	0.54
Satellite	chl	8.00	0.00	0.41	0.21	0.64	0.87	0.09	248.00	9.86	0.00	0.36	0.17	0.27	0.34
Satellite	chl	10.00	0.00	0.38	0.21	0.64	0.82	0.08	253.00	9.99	0.00	0.33	0.17	0.27	0.37
eReefs	chl	3.00	6.00	0.34	0.23	0.43	0.13	0.02	221.00	6.09	0.00	0.09	0.07	0.11	0.46
eReefs	chl	4.00	6.00	0.34	0.23	0.43	0.12	0.02	239.00	6.03	0.00	0.09	0.07	0.10	0.47
eReefs	chl	3.00	5.00	0.34	0.23	0.43	0.14	0.02	221.00	6.09	0.00	0.09	0.08	0.11	0.46
eReefs	chl	2.00	6.00	0.35	0.23	0.43	0.13	0.02	195.00	5.72	0.00	0.09	0.07	0.11	0.45
eReefs	chl	3.00	7.00	0.35	0.23	0.43	0.12	0.02	221.00	5.88	0.00	0.09	0.07	0.10	0.46
Satellite	nap	3.00	2.00	1.76	0.95	0.90	0.35	0.02	500.00	15.62	0.00	0.94	0.50	0.31	0.50
Satellite	nap	2.00	2.00	1.81	0.96	0.91	0.35	0.02	491.00	14.78	0.00	0.97	0.50	0.27	0.52
Satellite	nap	7.00	2.00	1.88	1.00	0.93	0.34	0.02	514.00	13.50	0.00	1.04	0.54	0.22	0.52
Satellite	nap	8.00	2.00	1.88	1.01	0.93	0.33	0.02	514.00	13.35	0.00	1.03	0.54	0.21	0.54
Satellite	nap	9.00	2.00	1.88	1.01	0.93	0.33	0.02	514.00	13.43	0.00	1.01	0.53	0.20	0.56
eReefs	nap	1.00	4.00	2.34	1.36	0.68	0.10	0.03	96.00	3.12	0.00	0.76	0.50	0.08	0.08
eReefs	nap	1.00	3.00	2.37	1.37	0.68	0.12	0.04	96.00	3.11	0.00	0.87	0.51	0.08	0.08
eReefs	nap	11.00	4.00	2.57	1.28	0.69	0.07	0.02	246.00	4.48	0.00	0.55	0.39	0.07	0.17
eReefs	nap	12.00	4.00	2.57	1.28	0.69	0.07	0.02	246.00	4.49	0.00	0.55	0.39	0.07	0.17
eReefs	nap	10.00	4.00	2.57	1.28	0.69	0.07	0.02	246.00	4.45	0.00	0.56	0.39	0.07	0.16
Satellite	sd	6.00	0.00	4.64	3.50	0.43	0.16	0.02	217.00	10.16	0.00	0.74	0.54	0.34	0.42
Satellite	sd	4.00	0.00	4.73	3.59	0.43	0.16	0.01	207.00	11.42	0.00	0.70	0.54	0.40	0.45
Satellite	sd	7.00	0.00	4.63	3.51	0.43	0.15	0.02	224.00	10.00	0.00	0.73	0.55	0.33	0.41
Satellite	sd	10.00	0.00	4.62	3.50	0.43	0.15	0.02	231.00	9.27	0.00	0.75	0.57	0.29	0.38
Satellite	sd	5.00	0.00	4.70	3.56	0.43	0.16	0.01	211.00	11.05	0.00	0.70	0.53	0.38	0.44
eReefs	sd	5.00	1.00	13.46	11.62	2.36	1.29	0.12	185.00	10.81	0.00	6.61	5.12	0.38	0.39
eReefs	sd	4.00	1.00	13.13	11.31	2.37	1.23	0.12	196.00	10.39	0.00	6.47	4.92	0.35	0.37
eReefs	sd	6.00	1.00	13.53	11.69	2.37	1.30	0.13	185.00	10.40	0.00	6.43	4.96	0.38	0.41
eReefs	sd	8.00	1.00	13.91	12.00	2.38	1.38	0.13	185.00	10.31	0.00	6.39	4.97	0.40	0.45
eReefs	sd	7.00	1.00	13.75	11.88	2.39	1.33	0.13	185.00	10.30	0.00	6.45	4.98	0.38	0.42

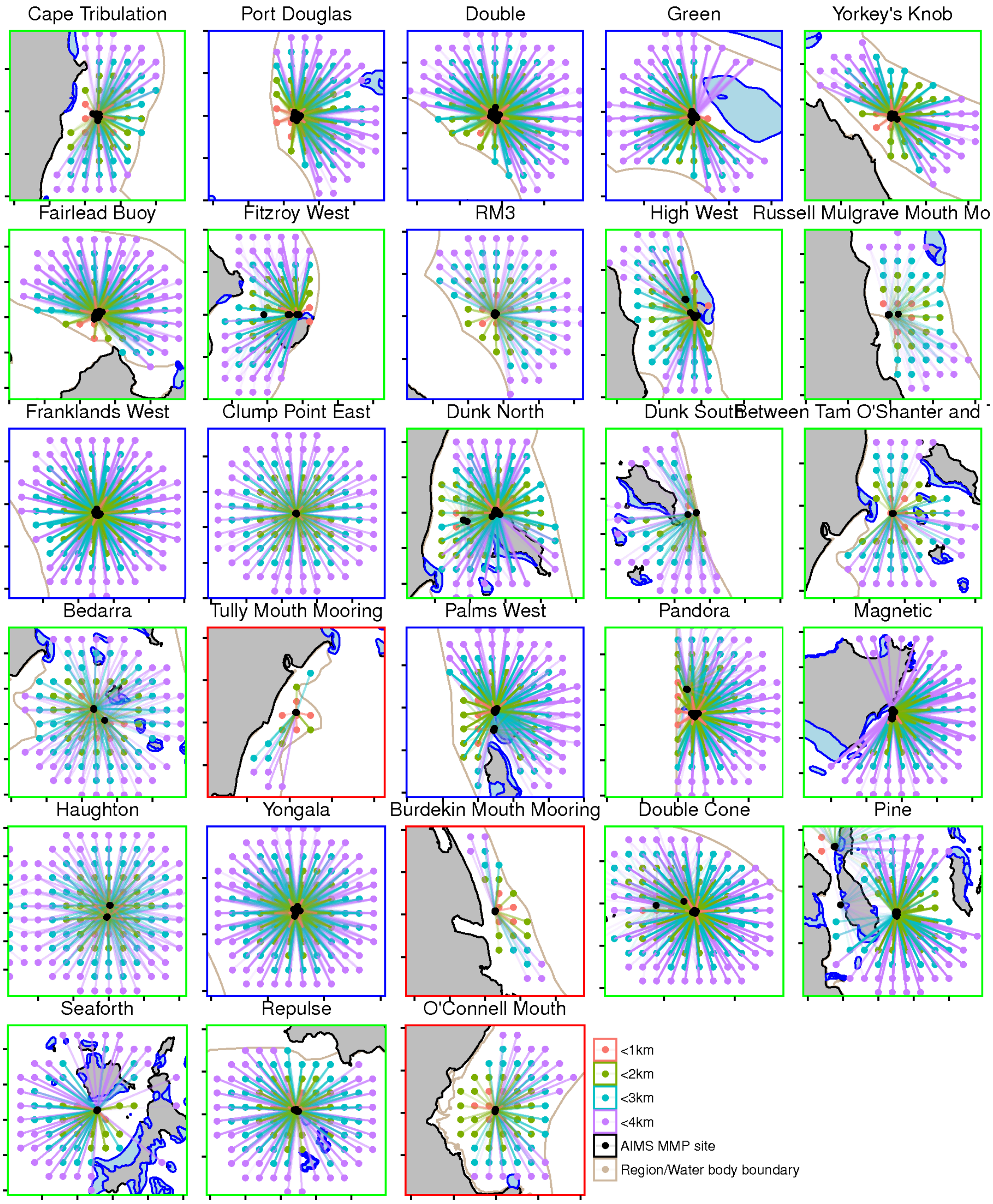


Figure 19: Location of Satellite cells within 5km of AIMS niskin samples. Panel borders represent water bodies (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

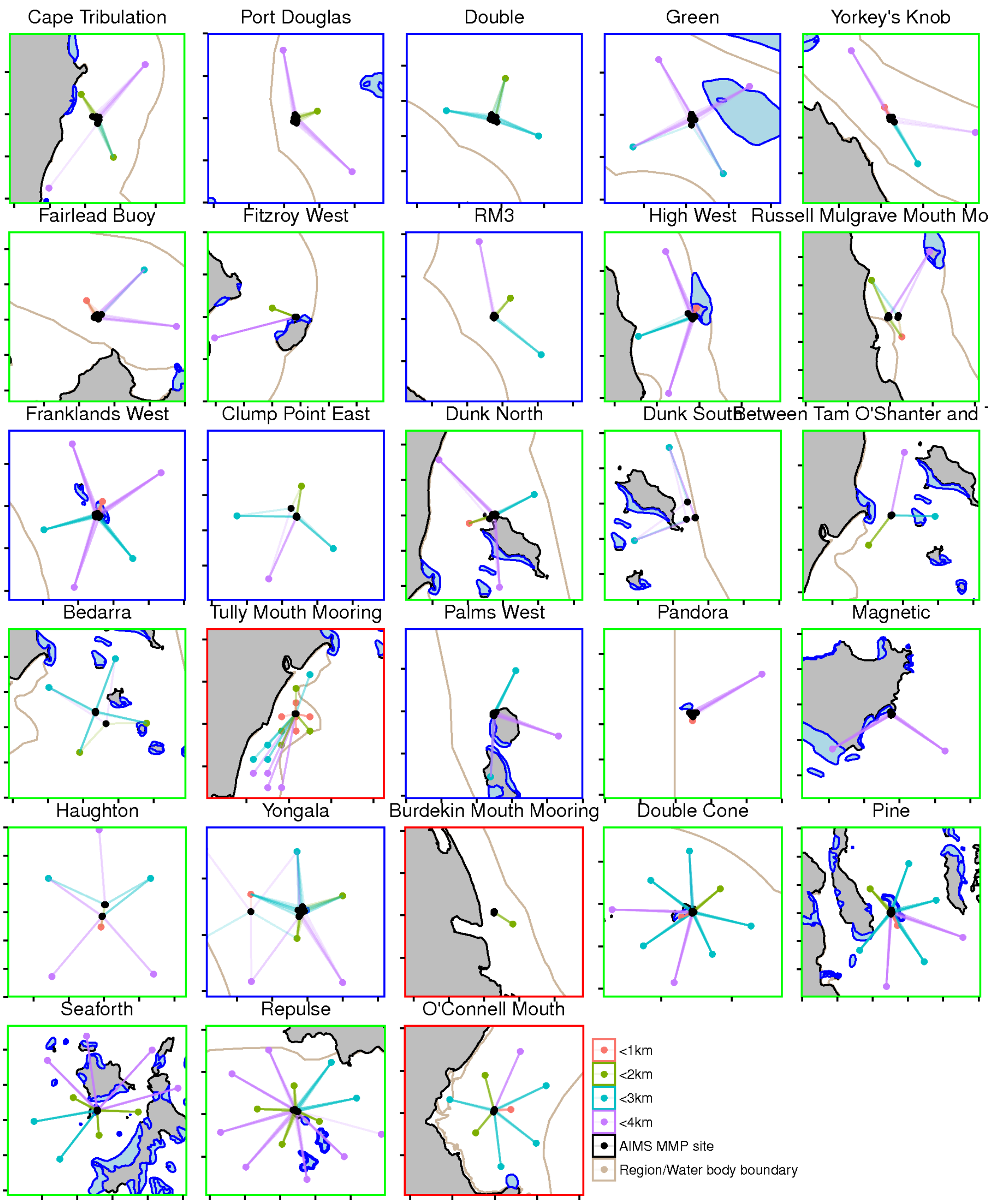


Figure 20: Location of eReefs cells within 5km of AIMS niskin samples. Panel borders represent water bodies (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

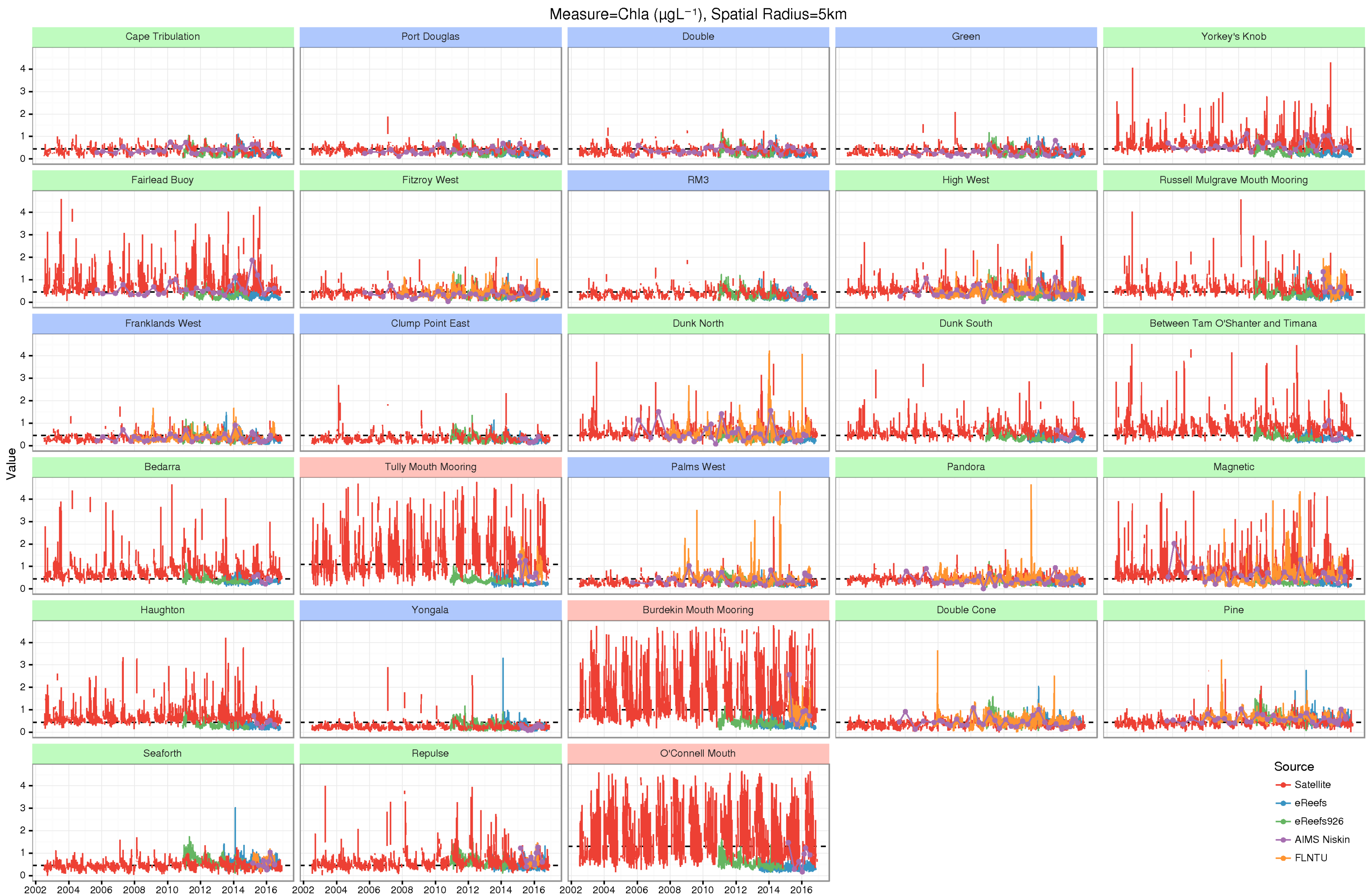


Figure 21: Temporal patterns in Chlorophyll-a within 5km of each AIMS MMP sampling site for eReefs, Satellite and AIMS insitu and FLNTU logger sources. Horizontal dashed line represents the guideline value. Title backgrounds represent water bodies (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

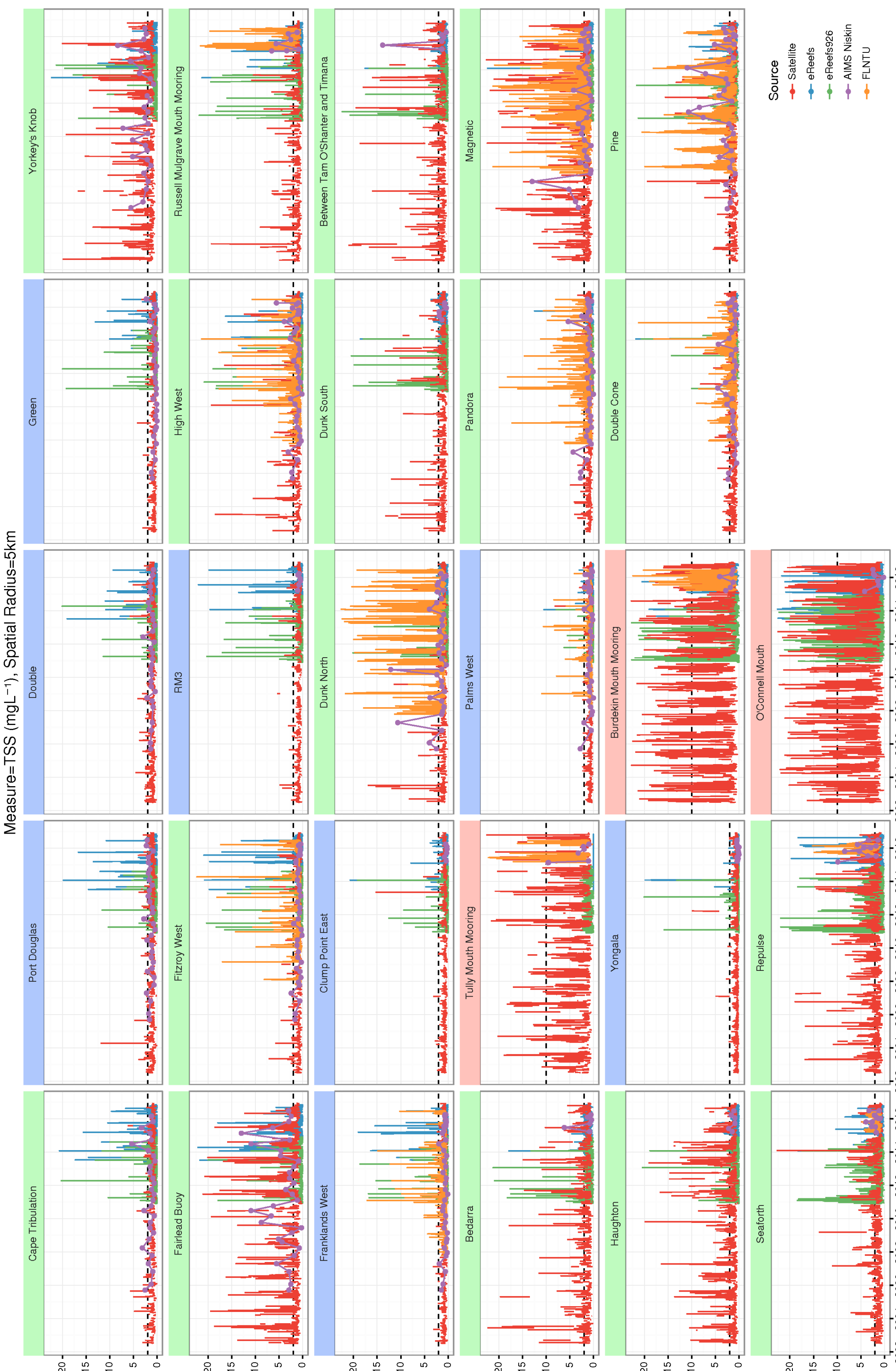


Figure 22: Temporal patterns in TSS within 5km of each AIMS MMP sampling site for eReefs, Satellite and AIMS insitu and FLNTU logger sources. Horizontal dashed line represents the guideline value. Title backgrounds represent water bodies (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

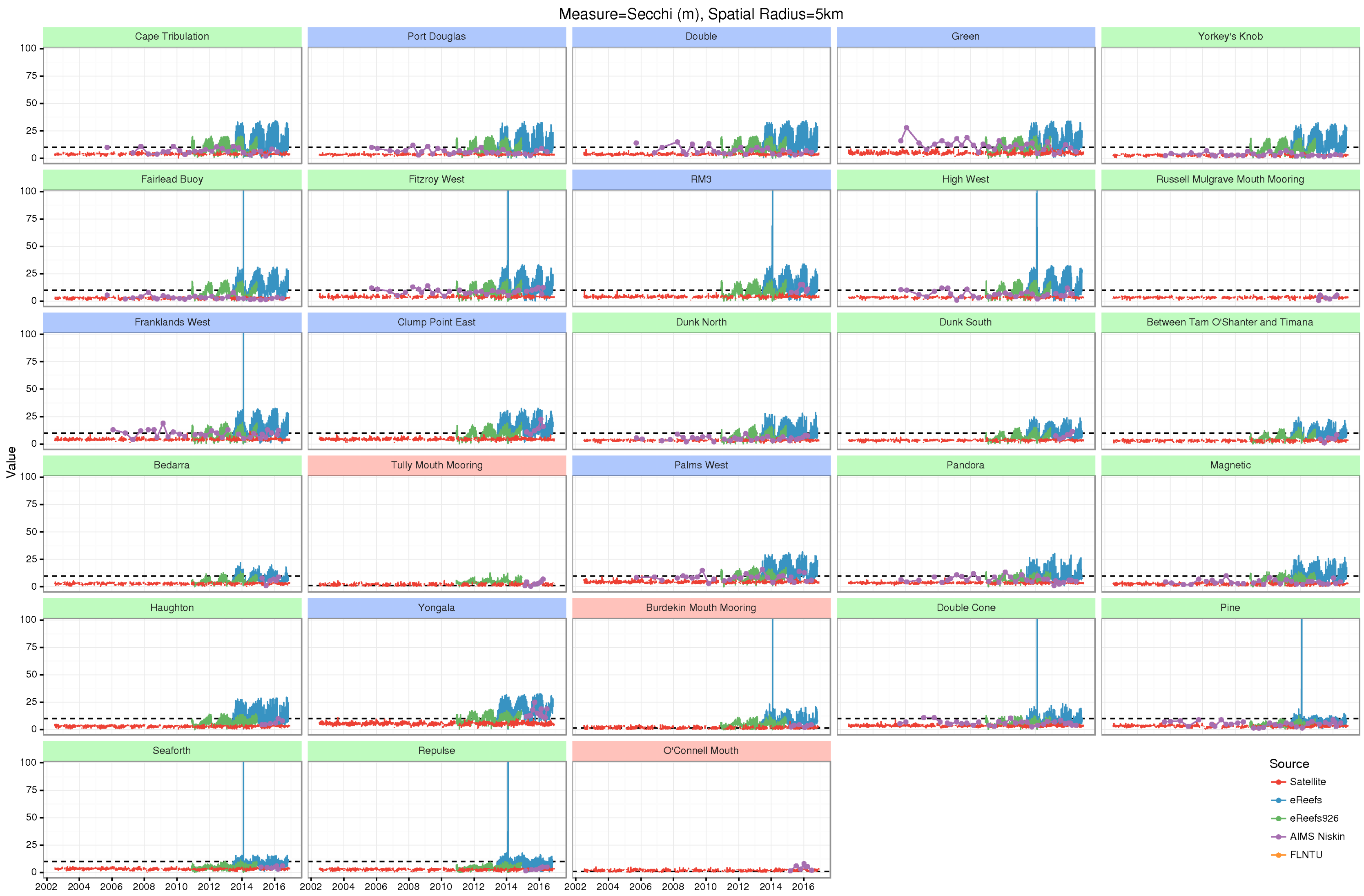


Figure 23: Temporal patterns in Secchi Depth within 5km of each AIMS MMP sampling site for eReefs, Satellite and AIMS insitu and FLNTU logger sources. Horizontal dashed line represents the guideline value. Title backgrounds represent water bodies (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

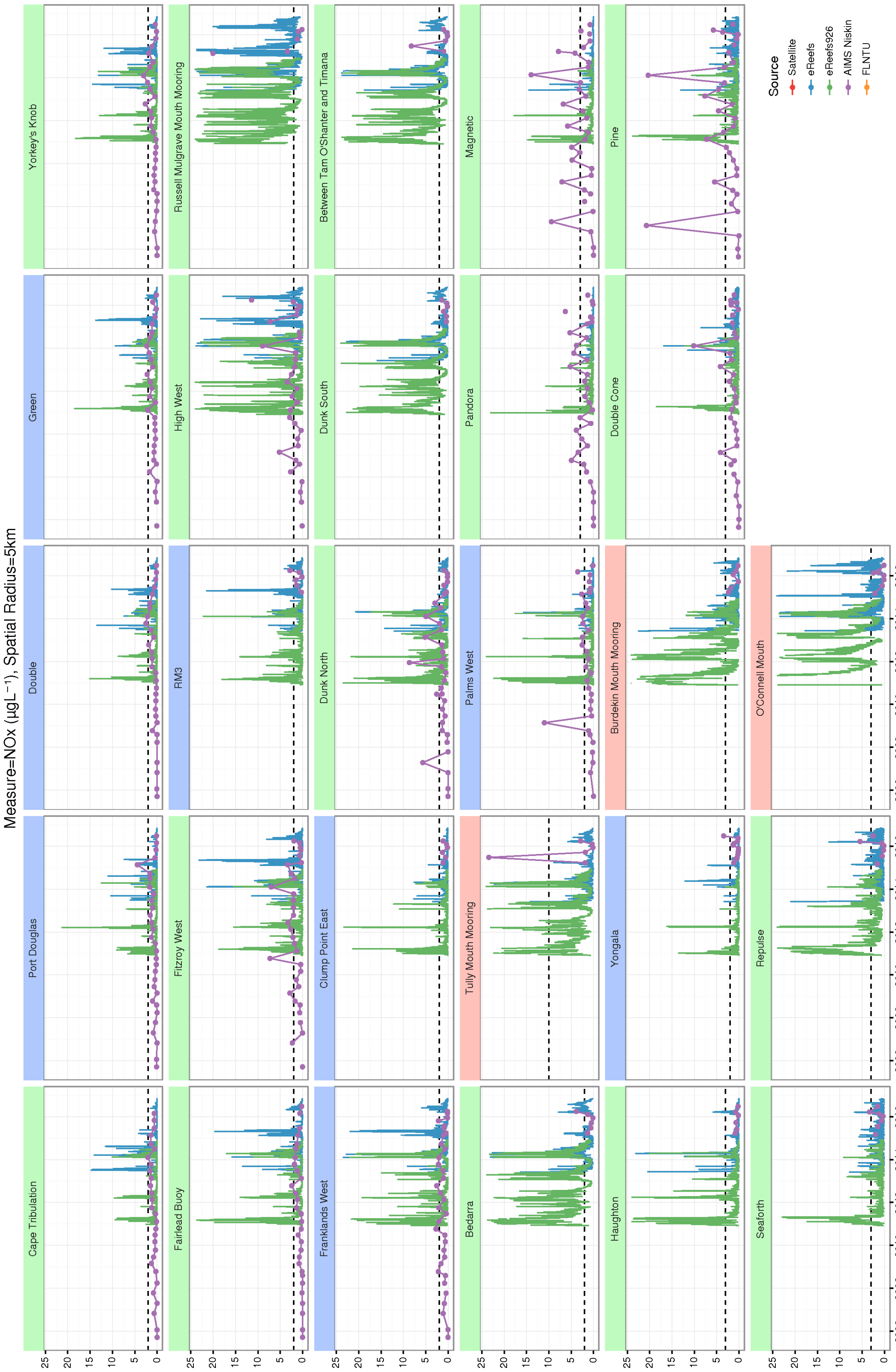


Figure 24: Temporal patterns in NOx within 5km of each AIMS MMP sampling site for eReefs, Satellite and AIMS insitu and FLNTU logger sources. Horizontal dashed line represents the guideline value. Title backgrounds represent water bodies (Red: Enclosed Coastal, Green: Open Coastal, Blue: Midshelf).

5. INDEX METRICS

5.1 Theoretical framework

Each individual indicator (or sub-indicator) addresses a different aspect of the state of an ecosystem. Hence, even a modest number of (sub)indicators will yield multiple perspectives on ecosystem health. Capturing the essence of the ecosystem health or an indicator thereof, necessitates integrating (aggregating) each of these perspectives together into a single index. There are numerous methods that have been applied to index aggregation, the most popular of which are itemized by Fox (2013) and described and evaluated in the context of water quality indices by either Walsh and Wheeler (2012) (from the perspective of cost benefit analyses) or Whittaker et al. (2012).

5.1.1 Multivariate health indicators

Motivated by the need to integrate multiple disparately scaled ecological variables together in the absence of any normalizing information (such as benchmarks, guidelines or thresholds, see Section 5.1.2), a variety of predominantly multivariate analyses have been used in the generation of ecosystem health indices. However, Whittaker et al. (2012) cautioned that since the incorporated weights are all exclusively informed by the statistical properties of the constituent indicator data, if these statistical properties did not coincide with expert knowledge of the relative importance of the indicators, then the resulting indices are likely to be poor.

As an alternative, Whittaker et al. (2012) suggest the Malmquist index. The computational details of the Marlmquist index are rather complex and since this method does not appear to have been adopted by any report cards, we will restrict our description to just a brief overview. Whittaker et al. (2012)'s proposed version of the Malmquist index calculates pairwise ratios of indicator distances from a multivariate benchmark curve. The benchmark curve (a form of indifference curve), is a multivariate curve defined by the lower boundary of a convex hull of all indicator values and is thus derived entirely from the observed data. Using simulated data with manufactured statistical complications (heterogeneity and temporal autocorrelation), Whittaker et al. (2012) demonstrated that the Malmquist index out performs indices based on principal components analysis and suggested other statistical methods would have similar shortcomings.

5.1.2 Thresholds

The absolute value of an indicator is rarely a meaningful assessment of ecosystem health assessments. Nor are the statistical properties of a time series necessarily a good basis for normalizing indicators or representing the objectives. What constitutes a 'good' or 'poor' level is likely to vary according to indicator, the ecosystem (e.g. freshwater, estuarine or marine) as well as the geographical and temporal (e.g. pre-industrial or current, seasonal) context. Another way to normalize the location (center) of indicators (if not the scale as well) that incorporates both knowledge about the ecological basis of the indicator and the objectives that they address is to express the indicators relative to benchmarks.

Benchmarks are typically either reference or baseline conditions (sites or historic data representing relatively low disturbance 'healthy' conditions), threshold values (ecotoxicology tolerances representing the cusp of 'unhealthy conditions) or guideline values (derived from either historical quantiles or ecotoxicology). Thresholds and guideline values are typically peer reviewed and ecologically meaningful, yet their specificity varies from local to regional, national or international standards.

Whilst a 'distance to benchmark' approach does provides some level of standardization (Connolly et al., 2013), to be useful, not only should there be some form of homogenization in what the benchmark condition represents, the polarity of the distance should be well understood (Hijuelos and Reed, 2013) and the magnitude of the distance should be commensurate with position along a disturbance gradient. That is, there should be some consistency in what it means to be above or below a benchmark, and indeed what it means to be a certain distance from a benchmark. Ideally, benchmarks should also be locally relevant (Connolly et al., 2013) and consider seasonal variability (Coates et al., 2007; Hallett et al., 2012). Indeed, in a review of the methodologies used to set benchmarks, (Borja et al., 2012) demonstrated the importance of setting appropriate benchmarks from which to assess ecosystem quality by directly linking the inability of indices to detect impacts in ecosystems to inappropriate reference conditions.

It is also important that benchmarks align with objectives in order to ensure indicators are appropriate. For example, if an objective is to maintain sustainable stocks of a particular species of fish, a benchmarks that reflect either historical numbers or the numbers present at low pressure sites do not necessarily represent the level of sustainability.

Ecological monitors have long recognized the need to express ecosystem ratings as standardized scores and in terms that are more accessible to policy makers and the general public. Whilst initial applications focused on normalizing observed measures against subjective rating curves to yield dimensionless index values on the scale of [0,1] that could be readiby combined into a single understandable score or rating (e.g. Miller et al., 1986), more recent studies have explored formulations that compare observed measures to baseline, reference, objectives or guideline values (collectively, benchmarks) values (e.g. CCME, 2001; Hurley et al., 2012; Jones et al., 2013).

Connolly et al. (2013) reviewed the use of report cards for monitoring ecosystem health and tabulated the general properties of a range of methods employed across a many different monitoring programs. Rather than duplicate that information here, the current intention is to provide more specific details about the algorithms used across those programs.

5.1.3 Unifying indices

The Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI; CCME, 2001) incorporates comparisons to baseline based on scope (proportion of indicators that have one or more failures to meet objectives), frequency (proportion of all comparisons failing to meet objectives) and amplitude (the normalized degree to which failed comparisons exceed objectives).

$$
\begin{aligned}
F_1 &= 100.\left(\frac{Number\ of\ failed\ indicators}{Total\ number\ of\ indicators}\right)\\
F_2 &= 100.\left(\frac{Number\ of\ failed\ comparisons}{Total\ number\ of\ comparisons}\right)\\
F_3 &= \frac{100.E}{1+E}; \qquad E = \frac{\sum_{i=1}^{n} e_i}{n}; \qquad e_i = z_i.\left[\left(\frac{x_i}{benchmark_i}\right)^{\lambda_i} - 1\right]\\
z_i &= \begin{cases} 1 & \text{if ith comparison fails} \\ 0 & \text{otherwise} \end{cases}; \qquad \lambda_1 = \begin{cases} 1 & \text{If} < benchmark_i = \text{fail} \\ -1 & \text{If} > benchmark_i = \text{fail} \end{cases}\\
CCMEWQI &= 100 - \left(\frac{\sqrt{F_1^2 + F_2^2 + F_3^2}}{1.732}\right)
\end{aligned}
$$

where n is the number of comparisons.

Whilst the CCME WQI might serve its purpose in the context to which it is applied, it is unlikely to be a useful metric for any indices involving remote sensing data or indeed any situation with a reasonable large amount of data or indicators. One-third of the weighting of the metric is calculated on the proportion of indicators that failed. The more observations are collected, the more likely at least one of them will exceed the benchmark. Hence, this one-third will quickly approach a constant of 1 thereby reducing overall sensitivity. In addition, the one-third of the method that weighting on amplitude only does so with respect to failure - there is no degree of how well the data recedes the benchmark. Finally, unifying indices have very limited scope for propagating any uncertainty. Consequently, this metric of index computation will not be explored in this project.

Rather than calculate the proportion of all comparisons failing to meet objectives across all indicators (as in the frequency component of the CCME WQI), we could perform the calculation separately for each variable (measure). Whilst this formulation (Exceedence), is characterised by the same limitations as the above frequency component, since it is calculated separately for each variable, when aggregated together to form an overall indicator, there is greater potential for improved resolution and granularity.

5.1.4 Hierarchical indices

The CCME WQI unifies all indicators into a single index as part of the calculations. However, most other indices involve aggregating across a sets of individual indicator scores. There are numerous ways to formulate indicator scores based on deviations from a benchmark (see Table 5).

Importantly, these scores are typically calculated at the level of the observations. Most of the index formulations are relatively robust to outliers (since the scores are either on a scale that reduces the magnitude of outliers or are capped to a range) and thus aggregating together indicies is likely to be more robust than calculating indices from aggregated raw data. An exception to this might be in situations where benchmarks are defined in the context of a specific spatial or temporal aggregation (such as annual mean or median value).

The Binary method expresses a comparison to benchmark values on a binary compliance scale (1: complies with benchmark, 0: fails to comply) and whilst simple to perform and understand, this method results in indices that have the potential to be either under or overly sensitive (depending on how far observed values typically are from the benchmark). For example, at one extreme (when values are close to benchmark), slight changes yield dramatic fluctuations in scores. However, when values are substantially above or below the benchmark, even modest improvements or deterioration will be undetected. This rapid 'switching' behaviour is depicted by the stepped response curve.

Note, when aggregated via means, the Binary method is identical to the Exceedence method, except that uncertaintly propagation is slightly more straight forward via the Binary method.

In the State of the Great Lakes Report (EPA/EC, 1995), greater granuality is achieved via a panel of experts who classify each of six health indicators (aquatic community health, human health, habitat, contaminants, nutrients and economy) into four categories: poor, mixed/deteriorating, mixed/improving, good/restored. Similar expert rating or multi-category exceedance grading systems are employed in other report cards (e.g Tamar estuary Report Card; Attard et al., 2012) and whilst probably reasonably accurate, they are nonetheless highly dependent on the ongoing availability of a reasonably stable panel of independent experts.

The Benchmark and Worst Case Scenario method (see Table 5) employed by the Fitzroy Basin Report Card (Jones et al., 2013) reflects the degree of failure by scaling the difference between the observed values and benchmarks (20_{th} or 80_{th} percentile of long term data for values above and below the benchmark respectively) to the Worst Case Scenario values (10_{th} or 90_{th} percentiles respectively). The associated response curve demonstrates a linear decline in Score with increasing distance from the benchmark.

The Modified Amplitude method calculates the distance to benchmark on a logarithmic (base 2) scale. The base 2 logarithm represents ratios on a symmetric scale such that value that are twice and half the benchmark yield scores of the same magnitude (yet apposing signs), and has some inbuilt capacity to accommodate skewed data. The Modified Amplitude response curve illustrates how this method can be simultaneously relatively insensitive to slight fluctuations around the benchmark as well as sensitive to changes further away from the benchmark.

Contrastingly, the Logistic Amplitude method operates on a logit scale such that it is very sensitive to slight fluctuations close to the benchmark and becomes progressively less sensitive with increasing distance. This method is also automatically scaled to the range [0,1]. The steepness of the Logistic Amplitude response can also be controlled by a tuning parameter (T).

Water Quality indices (which are standardized measures of condition) are typically expressed relative to a guideline, threshold (see Table ?? on page ??) or benchmark. Of the numerous calculation methods available, those that take into account the distance from the threshold (i.e. incorporate difference-to-reference) rather than simply an indication of whether or not a threshold value has been exceeded are likely to retain more information as well as being less sensitive to small changes in condition close to the threshold.

The challenging aspect of distance (or amplitude) based index methodologies is that determinination what constitutes a large deviation from a benchmark depends on the scale of the measure. For example, a deviation of 10 units might be considered relatively large of turbidity (NTU) or salinity (ppt), yet might be considered only minor for the Chlorophyll-a ($\mu g/L$). In order to combine a range of such metrics together into a meaningful index, the individual scores must be expressed on a common scale. Whilst this is automatically the case for Binary compliance, it is not necessarily the case for distance based indices.

Table 5 describes and compares the formulations and response curves of the Binary compliance method as well as a number of amplitude (distance based) indexing methods.

The Modified Amplitude and Logistic Modified Amplitude are both based on a base 2 logarithm of the ratio of observed values to the associated be benchmark (see Table 5). This scale ensures that distances to the benchmark are symmetric (in that a doubling and halving equate to the same magnitude - yet apposing sign). Furthermore, the logarithmic transformation does provide some inbuilt capacity to accommodate log-normality (a common property of measured values).

By altering the sign of the exponent, the Modified Amplitude methods can facilitate stressors and responses for which a failure to comply with a benchmark would be either above or below the benchmark (e.g. NTU vs Secchi depth). Further modifications can be applied to accommodate measures in which the benchmark represents the ideal and deviations either above or below represent increasingly poorer conditions (e.g. pH and dissolved oxygen).

The raw Modified Amplitude scores are relatively insensitive to small fluctuations around a benchmarks and sensitivity increases exponentially with increasing distance to the benchmark. The resulting scores can take any value in the real line $[-\infty, \infty]$ and hence are not bounded[6] There are two broad approaches to scaling (see Table 5):

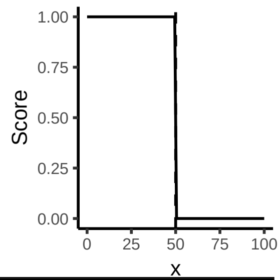
1. Capping and scaling: The log_2 scale can be capped to a range representing either a constant extent of change (e.g. twice and half the benchmark - a cap factor of 2) or else use historical quantiles (10th and 90th percentiles) to define the upper and lower bounds to which to cap the scale. Note historical quantiles are unavailable for the current application[7]. Thereafter, either can be scaled to the range [0,1] via a simple formula (see Table 5 III.Scaled).
2. Logistic Modified Amplitude: By expressing the scores on a logistic scale, the range of scores can be automatically scaled to range [0,1]. Moreover, this method allows the shape of the response curve to be customized for purpose. For example, the relative sensitivity to changes close or far from the benchmarks can be altered by a tuning parameter.

Rather than aggregating across sites before calculating indices, we would suggest that indices should be calculated at the site level. This is particularly important when different measures are measured at different sites. Spatial variability can be addressed via the use of a bootstrapping routine (see below). We would recommend that measurements collected throughout the reporting year be aggregated together into a single annual value. This is primarily because most water quality thresholds pertain specifically to annual averages rather than single time samples. Although it is possible to incorporate uncertainty due to temporal variability, the low sparse temporal frequency of sample collection is likely to yield uncertainty characteristics that will swamp the more interesting spatial sources of uncertainty.

Alternatively, if we relax the application of thresholds to individual observations, annual indices can be generated by aggregating observations level indices. When doing so, the Binary Compliance formulation aggregated via means will yield identical outcomes to the Exceedence formulation.

A useful metric for comparing the sensitivity of one indexing method over another is to take some representative longitudinal data and calculate indices based on the actual data as well as data that introduces progressively more noise.

Table 5: Formulations and example response curves for a variety of indicator scoring methods that compare observed values (x_i) to associated benchmark, thresholds or references values (B_i and dashed line). The Scaled Modified Amplitude Method can be viewed as three Steps: I. Initial Score generation, II. Score capping (two alternatives are provided) and III. Scaling to the range [0,1]. The first of the alternative capping formulations simply caps the Scores to set values (on a log_2 scale), whereas the second formulation (Quantile based, where $Q1$ and $Q2$ are quantiles) allows thresholds quantiles to be used for capping purposes. Dotted lines represent capping boundaries. In the Logistic Scaled Amplitude method, T is a tuning parameter that controls the logistic rate (steepness at the inflection point). For the purpose of example, the benchmark was set to 50.

Method	Formulation	Response curve
Binary compliance	$Score_i = \begin{cases} 1 & \text{if } x_i \leq B_i \\ 0 & \text{if } x_i \text{ else} \end{cases}$	

[6] Unbounded indices are difficult to aggregate, since items that have very large magnitude scores will have more influence on the aggregation than those items with scores of smaller magnitude. Furthermore, unbounded scores are difficult to convert into alphanumeric Grades. Consequently, the Scores need to be scaled before they can be converted to alphabetical grading scale.

[7] The use of historical quantiles makes the explicit assumption that the domain of expectations (from very good to very poor) is encapsulated within the historical data. For the eReefs model data, only three years of historical data are available. This is unlikely to be sufficient to represent the full spread of what we should consider our expectations - particularly when we acknowledge that the eReefs model data do not extend back as far as the 2010-2011 floods during which water quality conditions might be expected to be lower than the years to follow.

Table 5: Report Card indexing methods, continued

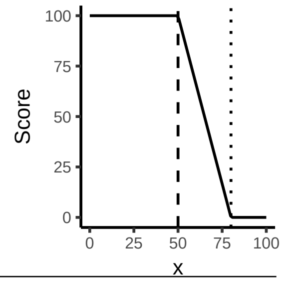
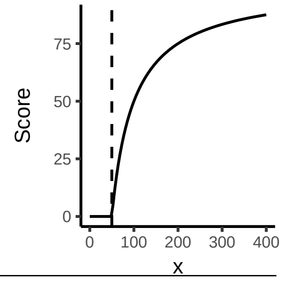
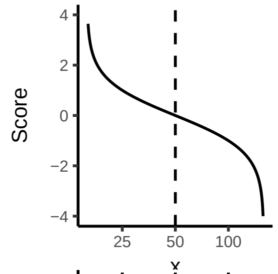
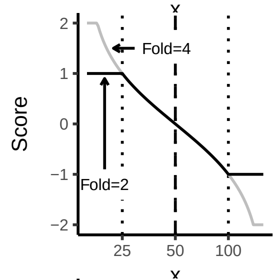
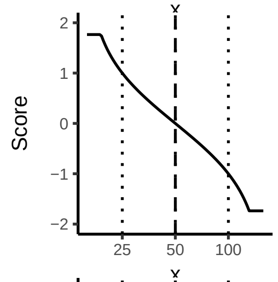
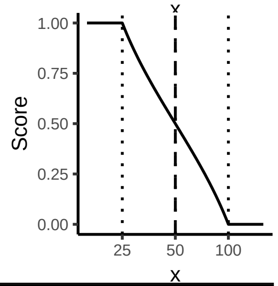
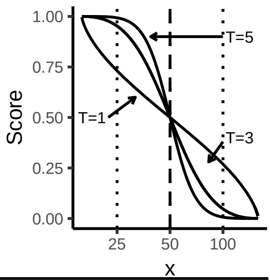
Method	Formulation	Response curve
Benchmark and WCS	$Score_i = \begin{cases} 100 & \text{if } x_i \leq B_i \\ 0 & \text{if } x_i \geq WCS_i \\ \left[1.0 - \left\lvert \frac{x_i - B_i}{WCS_i - B_i} \right\rvert\right].100 & \text{else} \end{cases}$	
Amplitude	$Score_i = \begin{cases} (\frac{x_i}{B_i})^{-1} & \text{if} > B_i = \text{fail} \\ (\frac{x_i}{B_i})^{1} & \text{if} < B_i = \text{fail} \end{cases}$ $Score_i = \frac{100 \times Score_i}{1 + Score_i}$	
Modified Amplitude	I. Raw (MAMP) $Score_i = \begin{cases} log_2(\frac{x_i}{B_i})^{-1} & \text{if} > B_i = \text{fail} \\ log_2(\frac{x_i}{B_i})^{1} & \text{if} < B_i = \text{fail} \end{cases}$	
	II. Fixed caps (Fold=2; [0.5,2]) (Fold=4; [0.25,4]) $Score_i = \begin{cases} log_2(1/2) & \text{if } Score_i < -1 \\ log_2(2/1) & \text{if } Score_i > 1 \\ Score_i & otherwise \end{cases}$	
	II. Quantile/extremes based caps ([15,170]) $Score_i = \begin{cases} log_2(\frac{Q1}{B_i})^{-1} & \text{if } x_i < Q1 \\ log_2(\frac{Q2}{B_i})^{-1} & \text{if } x_i > Q2 \\ Score_i & otherwise \end{cases}$	
	III. Scaled (Fixed: Fold=2) $Score_i = \frac{Score_i - min(Score_i)}{max(Score_i) - min(Score_i)}$	

Table 5: Report Card indexing methods, continued

Method	Formulation	Response curve
Logistic Scaled Modified Amplitude	Raw $Score_i = \begin{cases} log_2(\frac{x_i}{B_i})^{-1} & \text{if} > B_i = \text{fail} \\ log_2(\frac{x_i}{B_i})^{1} & \text{if} < B_i = \text{fail} \end{cases}$ $Score_i = \frac{1}{1+e^{Score_i.-T}}$	
Logistic	Raw $Score_i = \begin{cases} \frac{1}{1+e^{T.(x_i/B_i)}} & \text{if} > B_i = \text{fail} \\ \frac{1}{1+e^{-T.(x_i/B_i)}} & \text{if} < B_i = \text{fail} \end{cases}$	

Whilst the state of the water (or other environmental condition) might be of interest in its own right, it might also be of interest from the perspective of the ecosystem supported by the water. For example, turbidity might be considered to provide important insights into the light availabity within the ecosystem. As such, the variability in light availability (turbidity) might be a more influential ecological driver/pressure than the exact light level within any given time frame. Furthermore, sustained conditions might be more influential than rapidly fluctuating conditions. For example, two time windows could experience the same turbidity average and variance, yet these summaries could manifest from very different fluctuation patterns (one experiencing rapid fluctuations, and the other experiencing sustained periods of contrasting conditions).

One index that captures the pattern of fluctuations could be based on a metric that expresses the number of consecutive days in which a threshold has been exceeded as a proportion of number of days in the time window (e.g. 365 days).

$$Score_i = 1 - (n_i/N_i)$$

where n_i is the maximum number of consecutive time units in which $x_i > B_i$ and N_i is the number of time units in the i^{th} spatio-temporal window.

Unfortunately, such a formulation imposes some relatively difficult requirements on the data. Firstly, the time series within each window must be complete (no gaps), otherwise it is difficult to asses N_i. This requirement limits its use to only the eReefs modelled data as the Satellite data, AIMS insitu and AIMS FLNTU data have substantial time gaps. Secondly, as the formulation is based on summing up exceedences, it is likely to be as susceptable to the recognised insensitivities associated with binary compliance. Indeed, these sensitivities may well be further amplified. Furthermore, it is not responsive to the magnitude of exceedence.

The next section will explore the performance of the following index formulations:

- Binary compliance (Binary)
- Exceedence - proportion of observations exceeding the threshold (on large datasets, this will converge with Binaary compliance (Exceed)
- Maximum duration of exceedence (Max_Duration)
- Modified Amplitude (MAMP)
- Fixed Modified Amplitude (fMAMP)
- Fixed Scaled (x2,1/2) Modified Amplitude (fsMAMP)
- Fixed Scaled (x4,1/4) Modified Amplitude (fsMAMP4)

5.2 Index sensitivity

The sensitivity of a metric can be gauged by either:

- Quantitative exploration of the relationships between the metric and gradients of the underlying conditions that the metric should respond to. This approach requires very well defined gradients as well as a clear understanding and measures of what constitutes a relationship. By optimizing the metric(s) to these gradients, this approach has the potential to bias outcomes towards these gradients at the expense of generality to other gradients.
- Have experts (or end users) qualitatively gauge the outcomes of different metrics against expected trends and patterns. That is, do the outcomes align with end user expectations. Although this approach is equally subjective and potentially biased as the quantitative exploration, it does not necessitate formulating statistical cutoffs and associated artifacts.
- Explore the behaviour and characteristics of the metric when calculated on data simulated to represent a range of scenarios (altering location and spread). Whilst this approach will not necessarily select the 'best' metric, it does permit identification of the limitations and assumptions associated with different metrics.

The above approaches are not mutually exclusive. The current project will explicitly explore sensitivity via a simulation approach, yet will also encourage feedback as to whether final outcomes align with expectations. It should be noted that the current project is limited in sources of data and measured properties. A metric is purely a re-expression of data in order to enhance or highlight a signal. If the underlying data do not contain the expected signal, a signal will likewise be absent from any metrics.

To explore the performance and sensitivity of the various index computations for a range of data scenarios, data were simulated from Gamma distributions varying in mean (relative to a threshold) and variance and sample size. The Gamma distribution is parameterized by two shape parameters that can be expressed in terms of mean and variance (*Gamma*$(\mu^2/\sigma^2, \mu/\sigma^2)$).

For each threshold value (GL = 0.1,0.2,0.5,1,1,10,100) and sample size (R=10,100,1000), a set of 28 data scenarios where simulated (see Table 6 so as to represent a full spectrum of possible sampling outcomes. For each threshold/sample size and set combination, indices were calculated and aggregated for the simulated data. The extremes of these combinations are presented in Figures 25, 28 and 29, a more extensive set of Figures are in Appendix ??. For the set of simulations, the smaller the threshold, the more variable the samples relative to the threshold. Within each threshold, the set of 28 scenarios thereby represent combinations of varying mean and relative variability.

Table 6: Index performance and sensitivity data scenarios. Data in each group are drawn from Gamma distributions whose parameterizations are based on a mean and variance. In each case the mean is some multiple of the threshold (GL) value. Multiples of threshold that are less than 1 result in data with greatest density below the threshold value. Lower variances result in less varied data.

Grp	Mean	SD	Grp	Mean	SD	Grp	Mean	SD	Grp	Mean	SD
1	$\mu = 0.2GL$	$\sigma^2 = 0.1$	9	$\mu = 0.75GL$	$\sigma^2 = 0.1$	17	$\mu = 1.5GL$	$\sigma^2 = 0.1$	25	$\mu = 4GL$	$\sigma^2 = 0.1$
2	$\mu = 0.2GL$	$\sigma^2 = 0.2$	10	$\mu = 0.75GL$	$\sigma^2 = 0.2$	18	$\mu = 1.5GL$	$\sigma^2 = 0.2$	26	$\mu = 4GL$	$\sigma^2 = 0.2$
3	$\mu = 0.2GL$	$\sigma^2 = 0.3$	11	$\mu = 0.75GL$	$\sigma^2 = 0.3$	19	$\mu = 1.5GL$	$\sigma^2 = 0.3$	27	$\mu = 4GL$	$\sigma^2 = 0.3$
4	$\mu = 0.2GL$	$\sigma^2 = 0.5$	12	$\mu = 0.75GL$	$\sigma^2 = 0.5$	20	$\mu = 1.5GL$	$\sigma^2 = 0.5$	28	$\mu = 4GL$	$\sigma^2 = 0.5$
5	$\mu = 0.5GL$	$\sigma^2 = 0.1$	13	$\mu = 1GL$	$\sigma^2 = 0.1$	21	$\mu = 2GL$	$\sigma^2 = 0.1$			
6	$\mu = 0.5GL$	$\sigma^2 = 0.2$	14	$\mu = 1GL$	$\sigma^2 = 0.2$	22	$\mu = 2GL$	$\sigma^2 = 0.2$			
7	$\mu = 0.5GL$	$\sigma^2 = 0.3$	15	$\mu = 1GL$	$\sigma^2 = 0.3$	23	$\mu = 2GL$	$\sigma^2 = 0.3$			
8	$\mu = 0.5GL$	$\sigma^2 = 0.5$	16	$\mu = 1GL$	$\sigma^2 = 0.5$	24	$\mu = 2GL$	$\sigma^2 = 0.5$			

Figure 25: Simulated data and associated indices for threshold of 0.1 and very large sample sizes (R=1000). Samples represent high variability relative to threshold.

As expected, indices decline with increasing values relative to the threshold (as would be the case for Chl-a or TSS) with a generally linear response being the attribute sought in our specific context. Testing the responses of indices to various combinations allowed the identification of the most appropriate and robust index calculation method.

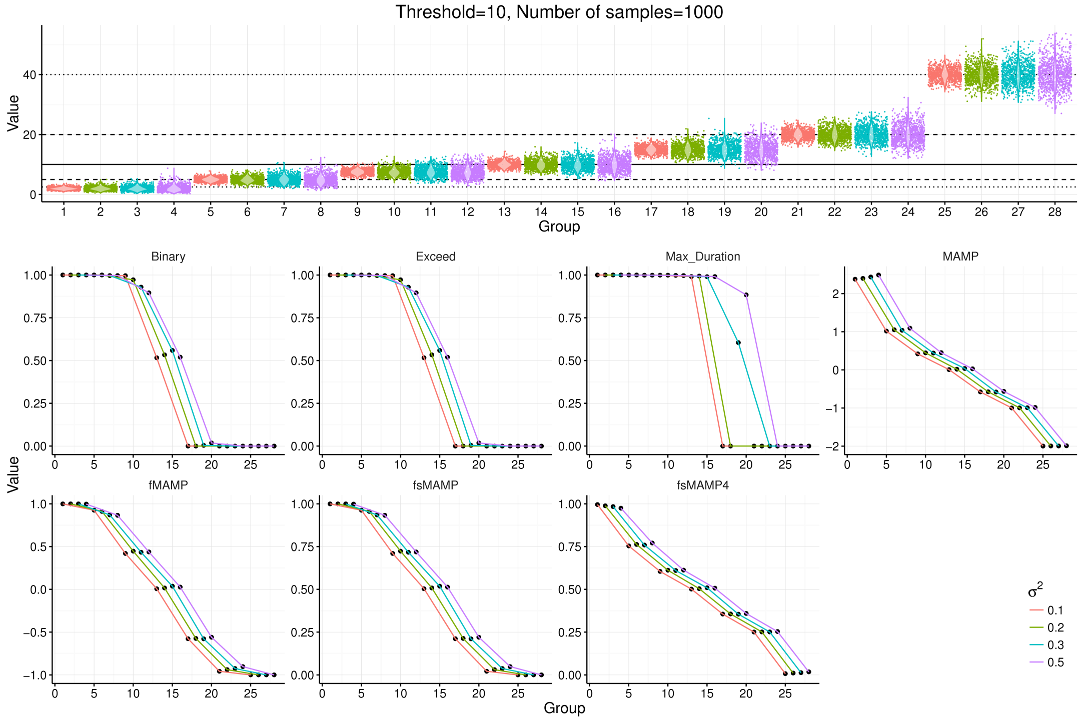


Figure 26: Simulated data and associated indices for threshold of 10 and very large sample sizes (R=1000).

When the number of samples and the relative sample variability is very large (e.g. fig. 25), with the exception of the the maximum duration of exceedance and the uncapped and unscaled modified amplitude (MAMP) methods, the different index calculation methods behave very similarly. However, as the variability of the samples declines relative to the threshold (e.g. compare figs. 25, 26 and 27), such that observations are predominantly within twice/half the threshold value, and data is predominantly distributed between the threshold value binary or frequency of exceedance methods both increasingly become simultaneously overly and under sensitive. The response curve of these metrics becomes less linear, whereas the linearity of the other metrics is maintained for a greater span of observation means. This is further exacerbated by small sample sizes (see fig.29).

Over all of the scenarios, the fsMAMP4 (Modified Amplitude capped at four times/quarter of threshold values) appears to be as linear or more linear than the fsMAMP (Modified Amplitude capped at twice/half), particularly as relative variability declines. However, the cost of this extended range of sensitivity, is that it is predominantly more sensitive at the extremes and less so (at least compared to fsMAMP) towards the mid-region (corresponding to values close to the threshold). Arguably, it is more desirable for an index to be most sensitive around the threshold (unless there is substantial uncertainty about the threshold value) and become progressively less sensitive at increasing distance from the threshold - the binary and exceedence metrics are the extreme cases of this.

The fixed capped modified amplitude (fsMAMP) index was considered the 'best' compromise between consistent sensitivity throughout the range of scenarios and the nature of data presented in exploratory data analyses (see Section ??). It should be noted that it is possible to modify the fsMAMP index metric to facilitate caps based on historical, biological or ecological parameters. It is also possible to define these parameters (an upper and lower capping) at any spatial/temporal/measure level so as to potentially build indices that are optimized for each measure. Such an exercise requires extensive expert knowledge to define and justify each of the parameters and is beyond the scope of the current project.

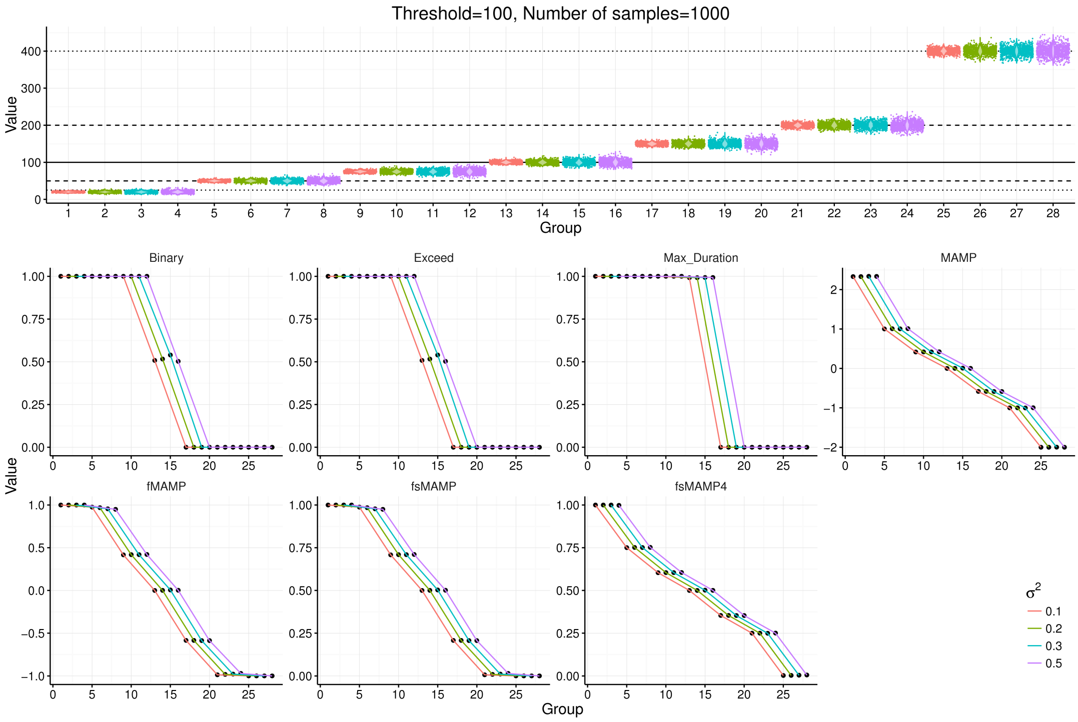


Figure 27: Simulated data and associated indices for threshold of 100 and very large sample sizes (R=1000).

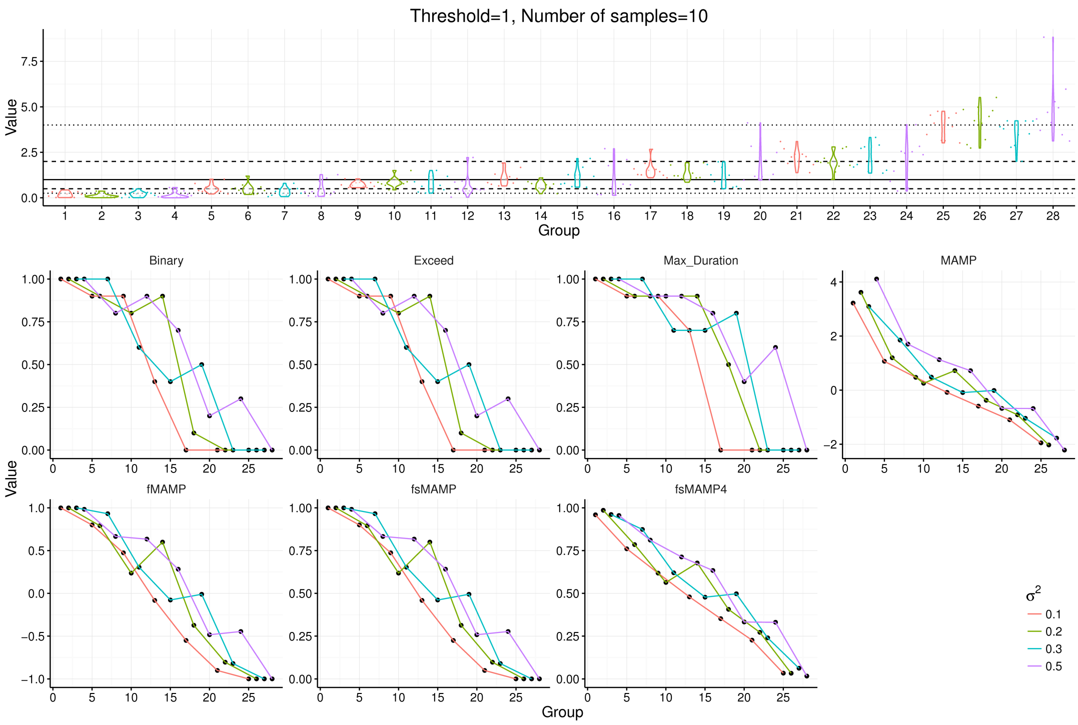


Figure 28: Simulated data and associated indices for threshold of 1 and large sample sizes (R=100).

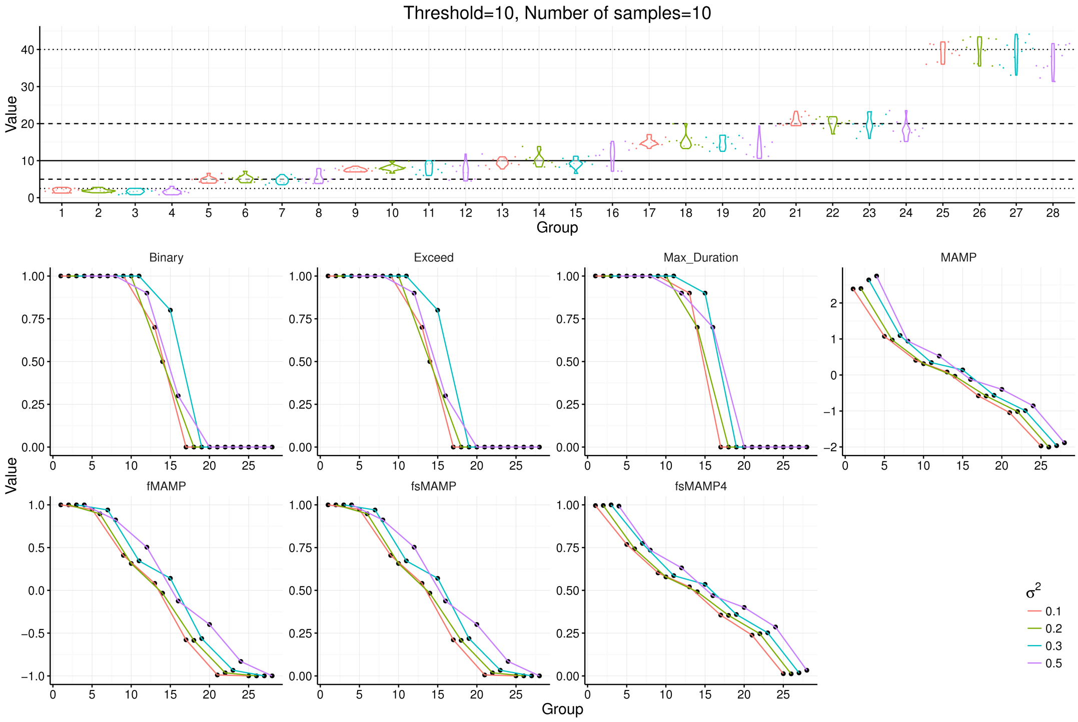


Figure 29: Simulated data and associated indices for threshold of 10 and small sample sizes (R=10).

5.2.0.1 Summary of simulation index sensitivity exploration

- Indices decline with increasing values relative to the thresholds (and for a given variability)
- Indices increase with increasing variability (since in Gamma distributions, this results in more values towards lower end)
- when R is very large, the different indicators behave similarly (except Max_Duration and MAMP)
- MAMP is more susceptable to outliers

5.3 Index explorations

Before data can be combined and aggregated across the various Sources (AIMS insitu, AIMS FLNTU, Satellite, eReefs and eReefs926) and Measures (Chlorophyll, TSS, Secchi depth and NOx), it is important that we evaluate the likely usefulness of each Source/Measure combination. For example, a Measure or Source that does not vary in both time and space is not considered very informative parameter.

Although an exploration of the patterns of spatial and temporal variation of the raw data does offer some insights into the usefulness of a parameter, it is variation in relation to expectations (thresholds) that are likely to be of greatest utility. For example, a parameter might vary substantially in time and or space and yet always be well above (or below) the threshold. In this situation (despite the apparent variability), with respect to the expectation domain, there is very little (if any) variability and thus the realised utility of the parameter is low (or else the threshold is inappropriate for the particular measure to which it is being applied).

Different parameters are measured on different scales or else have different natural background levels. Since variability (for example variance) is dependent on scale, parameters measured in larger units will typically exhibit more variability in absolute terms. Hence, in order to compare the relative utility of different parameters, it is necessary to either express variation relative to scale (such as coefficient of variation) or standardize the parameters. The scaled hierarchical index formations of Section 5.1.4 (such as Binary, fsMAMP, fsMAMP4 and logistic MAMP) are all a form of standardization which yeild scores on scales that are all bound [0,1].

The following three subsections will provide information to assist in the selection of:

- which Index formulation to adopt
- which Sources of data to use
- which Measures to include

5.3.1 Indices

Theoretical sensitivity investigation suggested that the fixed capped (half/twice threshold) Modified Amplitude (fsMAMP) is likely to be the best compromise between under and over sensitivity given the patterns of variance observed across and between the various Sources (AIMS insitu, AIMS FLNTU, Satellite, eReefs and eReefs926) and Measures (Chlorophyll, TSS, Secchi depth and NOx). The alternate approach is to explore and compare the patterns of the various index formulations in the context of both the raw collected data and expert expectations. Broadly speaking, we might expect that many water Quality parameters improve across the shelf with increasing distance from coastline. We might also expect some latitudinal patterns in which water quality generally improves along a south-north gradient with interruptions coinciding with outflow of major rivers.

To explore how the raw data are transformed into the various indices, it is useful to pair up 'before' and 'after' figures. Again, for the sake of brevity, we will focus on the same data that featured in Figure 1 (Chlorophyll-a from Wet Tropics, Open Coastal). Figures 30 – 34 illustrate the associations between the site means (subfigure a) and three of the major index candidates (b: Binary, c: fsMAMP and d: fsMAMP4) for each of the Sources of data (AIMS insitu, AIMS FLNTU, Satellite, eReefs and eReefs926). In these figures, purple and blue lines represent annual means and within year Generalized Additive Model (Wood, 2006) respectively and help highlight inter- and intra-annual variation[8].

Inter and Intra annual variation is greatest in the Binary index method for each data Source[9]. Whilst this method does illustrate sensitivity, the values of the index do not contain any context about the magnitude of values relative to the threshold. That is, it is not possible to distinguish situations in which all observations are just under (or over) the threshold from when they are substantially under (or over) the threshold. In this way, the index has the potential to be under-sensitive to magnitude, yet very sensitive to change around the threshold. For each of the Sources (except AIMS insitu for which data are too sparse), the relative magnitude of fluctuations in the Binary index (subfigure b) appears to be substantially greater than the relative magnitude of fluctuation in the observed data (subfigure a). These patterns of relative variability might imply that the Binary index is over-sensitive.

By contrast, the fsMAMP4 (capped at four times and one-forth threshold, subfigures d) could be interpreted as under-sensitive - particularly for the Satellite data (which has highly variable observations). The fsMAMP (twice/half

[8] GAMs not performed for AIMS insitu data due to a lack of data over which to estimate splines

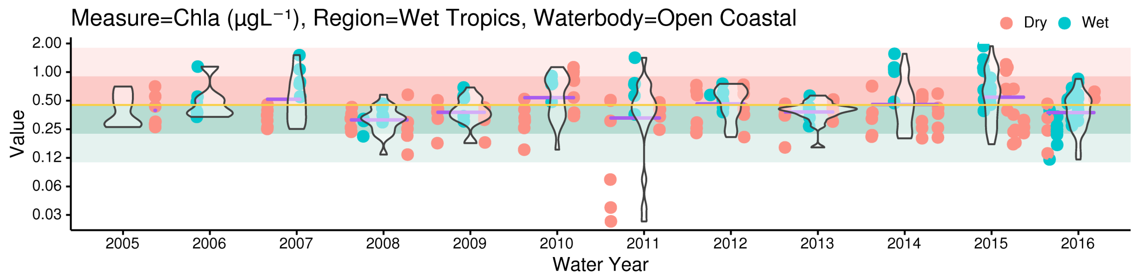
[9] this pattern also persists across all Zones (Region/Water body) and Measures - although other Measures and Zones not provided here to reduce space.

threshold) appears to in between these two extremes and thus could be considered a reasonable comprimise between over and under sensitivity.

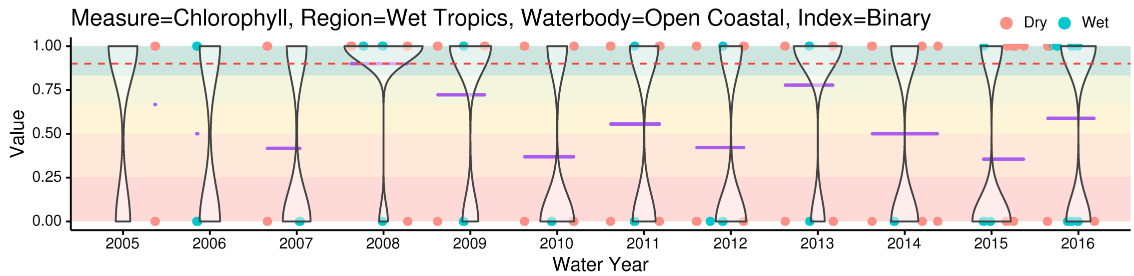
Spatial representations for Wet Tropics Open Coastal Chlorophyll-a (figs. 35 – 38) and Dry Tropics Midshelf Chlorophyll-a (figs. 39 – 43) offer similar assessments - that fsMAMP provides a reasonable compromise between the potentially under and over sensitive fsMAMP4 and Binary formulations.

Time series of annually aggregated observations and associated annually aggregated indices (figs. 44 – 48) provide simplified representations of the overall spatio-temporal patterns. As with the temporal and spatial representations, the fsMAMP index consistently manifests between the Binary and fsMAMP4 formulations.

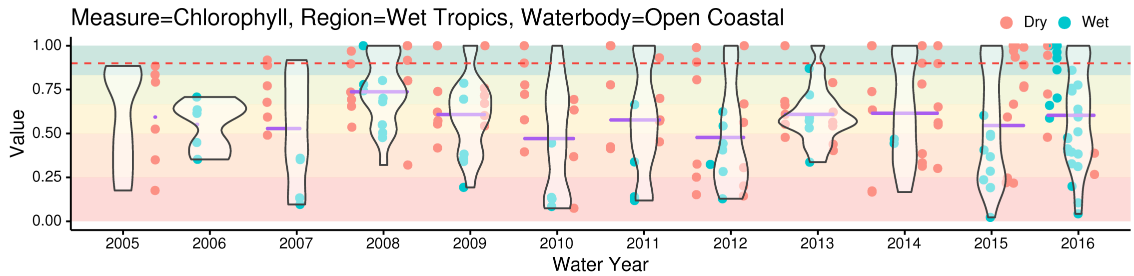
a) AIMS insitu site means



b) AIMS insitu site mean Binary



c) AIMS insitu site mean fsMAMP



d) AIMS insitu site mean fsMAMP4

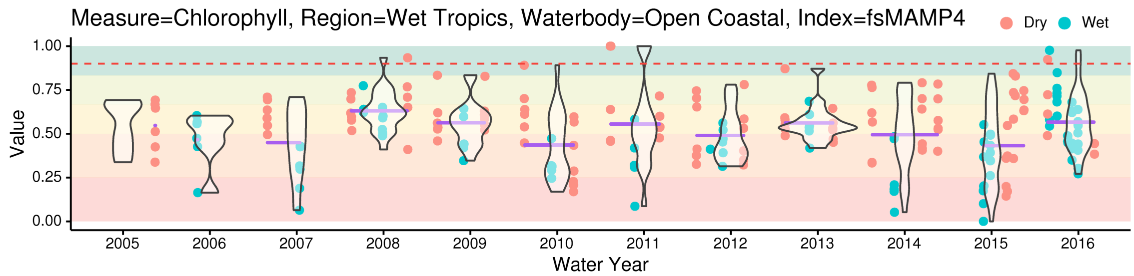
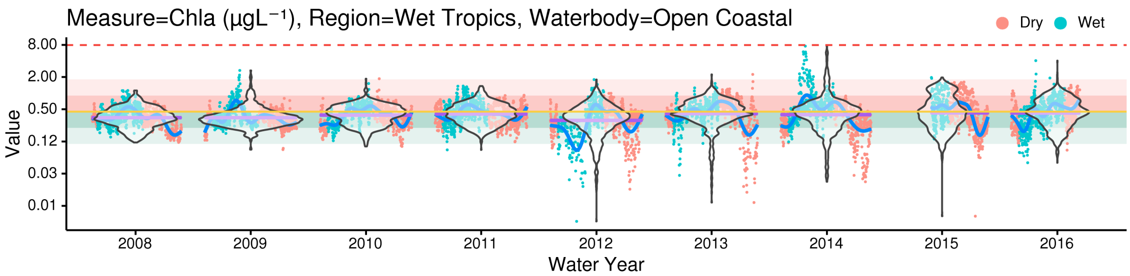
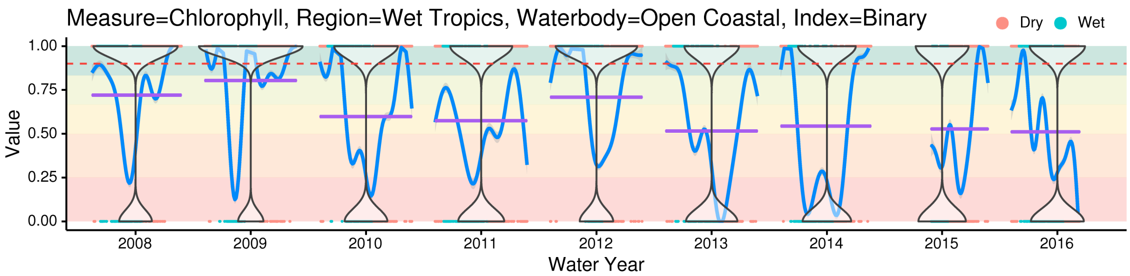


Figure 30: Temporal distribution of AIMS insitu Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Red and Blue symbols represent samples collected in Dry and Wet seasons respectively. Green and red shaded banding on a) respectively represent half and twice threshold value (50% shading) and one-forth and four times threshold value (30% shading). Traffic-light banding on b-d) indicates simple 5-level color scheme. Purple lines represent annual means.

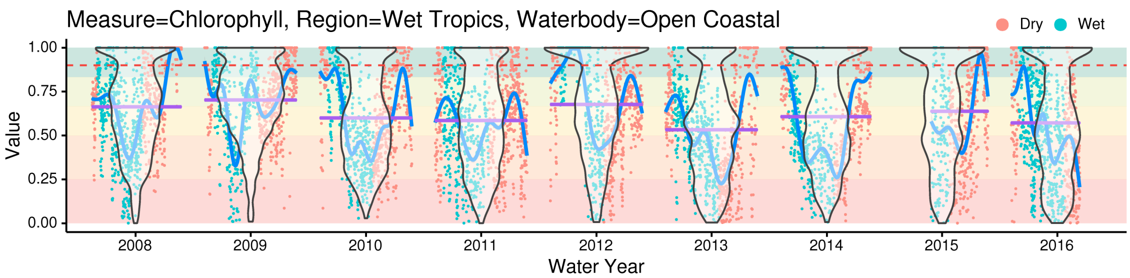
a) AIMS FLNTU raw site means



b) AIMS FLNTU site mean Binary



c) AIMS FLNTU site mean fsMAMP



d) AIMS FLNTU site mean fsMAMP4

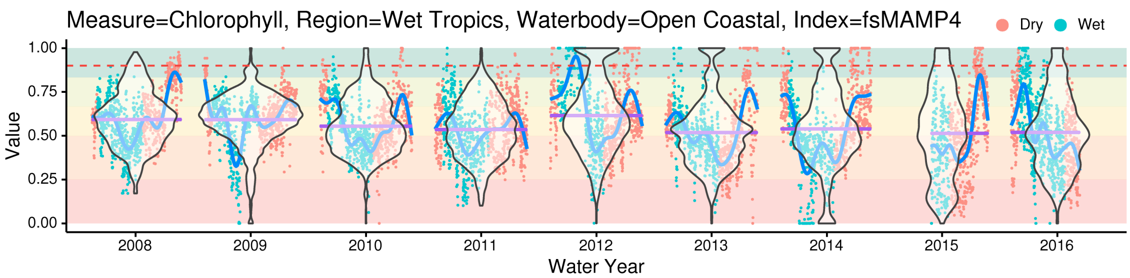
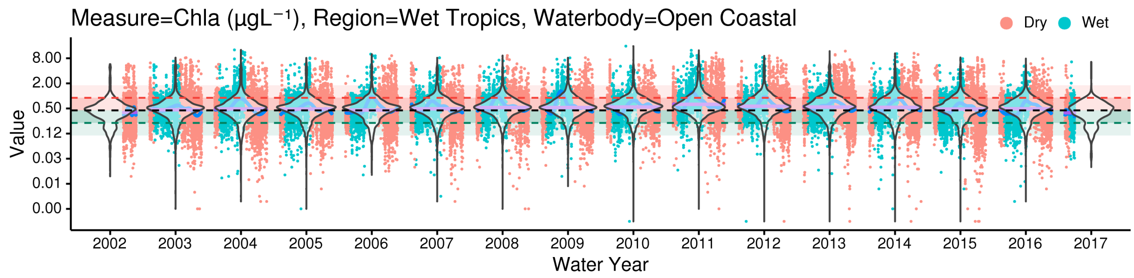
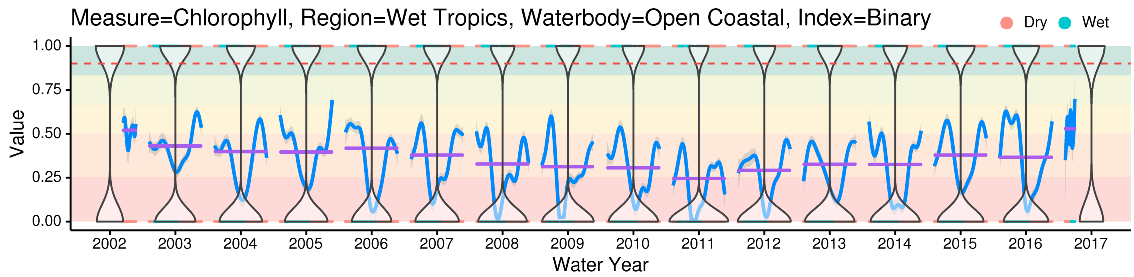


Figure 31: Temporal distribution of AIMS FLNTU Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Red and Blue symbols represent samples collected in Dry and Wet seasons respectively. Green and red shaded banding on a) respectively represent half and twice threshold value (50% shading) and one-forth and four times threshold value (30% shading). Traffic-light banding on b-d) indicates simple 5-level color scheme. Purple lines represent annual means.

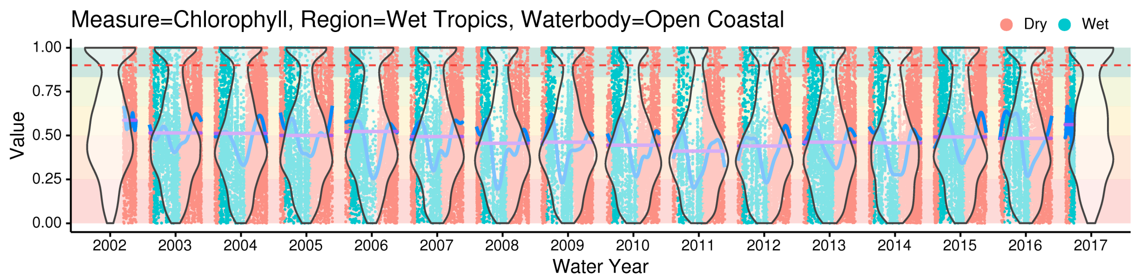
a) Satellite raw site means



b) Satellite site mean Binary



c) Satellite site mean fsMAMP



d) Satellite site mean fsMAMP4

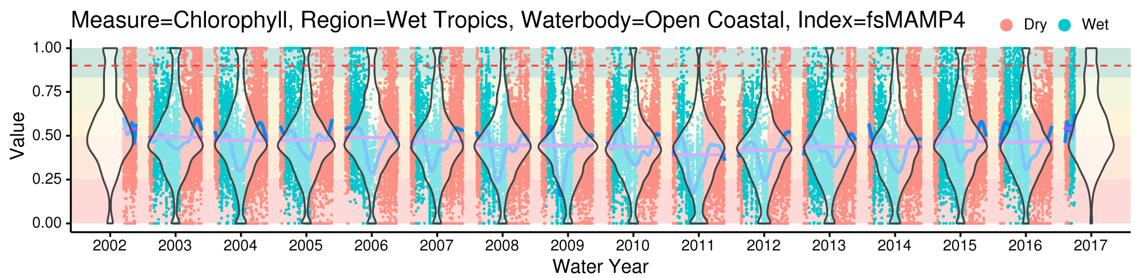
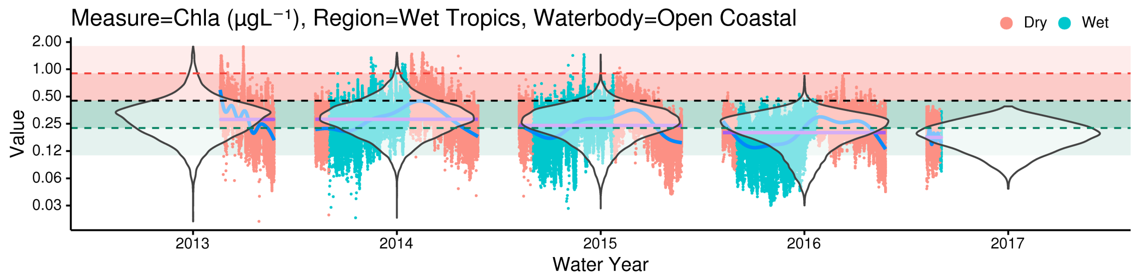
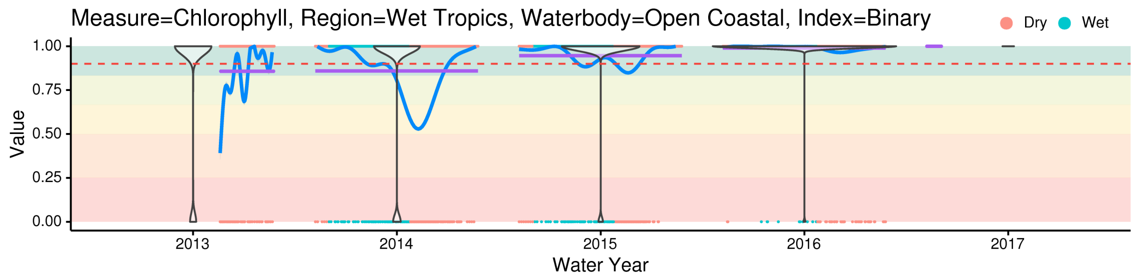


Figure 32: Temporal distribution of Satellite Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Red and Blue symbols represent samples collected in Dry and Wet seasons respectively. Green and red shaded banding on a) respectively represent half and twice threshold value (50% shading) and one-forth and four times threshold value (30% shading). Traffic-light banding on b-d) indicates simple 5-level color scheme. Purple lines represent annual means.

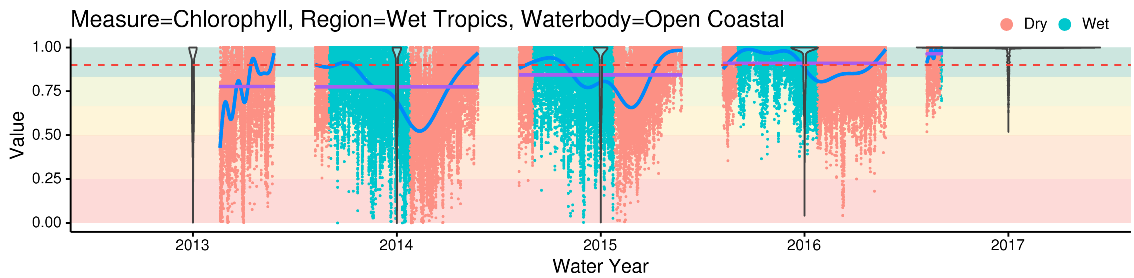
a) eReefs raw site means



b) eReefs site mean Binary



c) eReefs site mean fsMAMP



d) eReefs site mean fsMAMP4

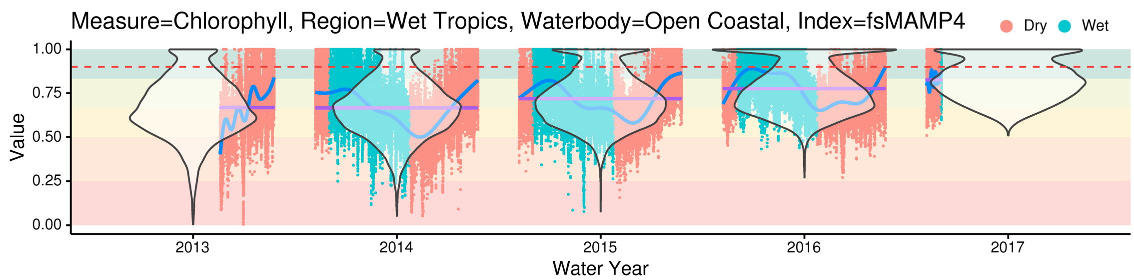
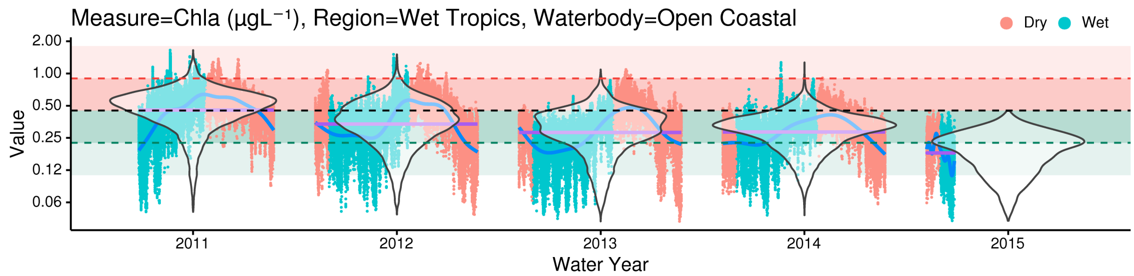
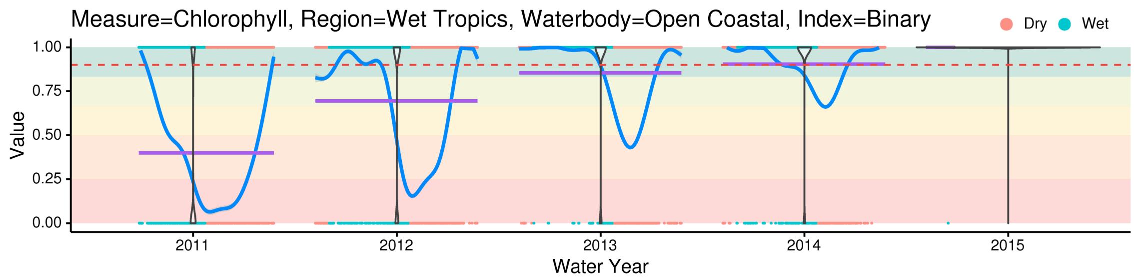


Figure 33: Temporal distribution of eReefs Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Red and Blue symbols represent samples collected in Dry and Wet seasons respectively. Green and red shaded banding on a) respectively represent half and twice threshold value (50% shading) and one-forth and four times threshold value (30% shading). Traffic-light banding on b-d) indicates simple 5-level color scheme. Purple lines represent annual means.

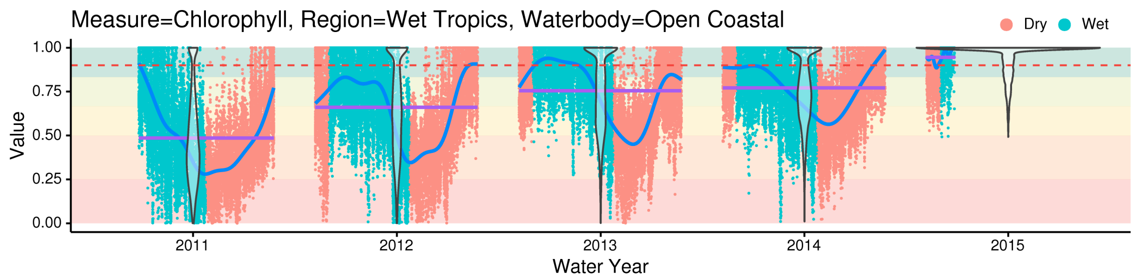
a) eReefs926 raw site means



b) eReefs926 site mean Binary



c) eReefs926 site mean fsMAMP



d) eReefs926 site mean fsMAMP4

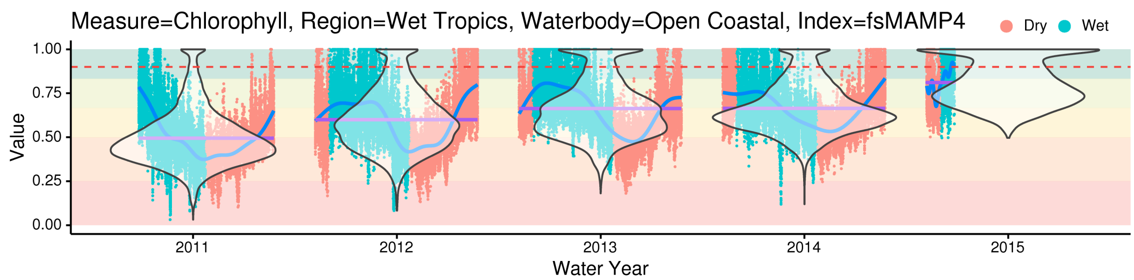


Figure 34: Temporal distribution of eReefs926 Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Red and Blue symbols represent samples collected in Dry and Wet seasons respectively. Green and red shaded banding on a) respectively represent half and twice threshold value (50% shading) and one-forth and four times threshold value (30% shading). Traffic-light banding on b-d) indicates simple 5-level color scheme. Purple lines represent annual means.

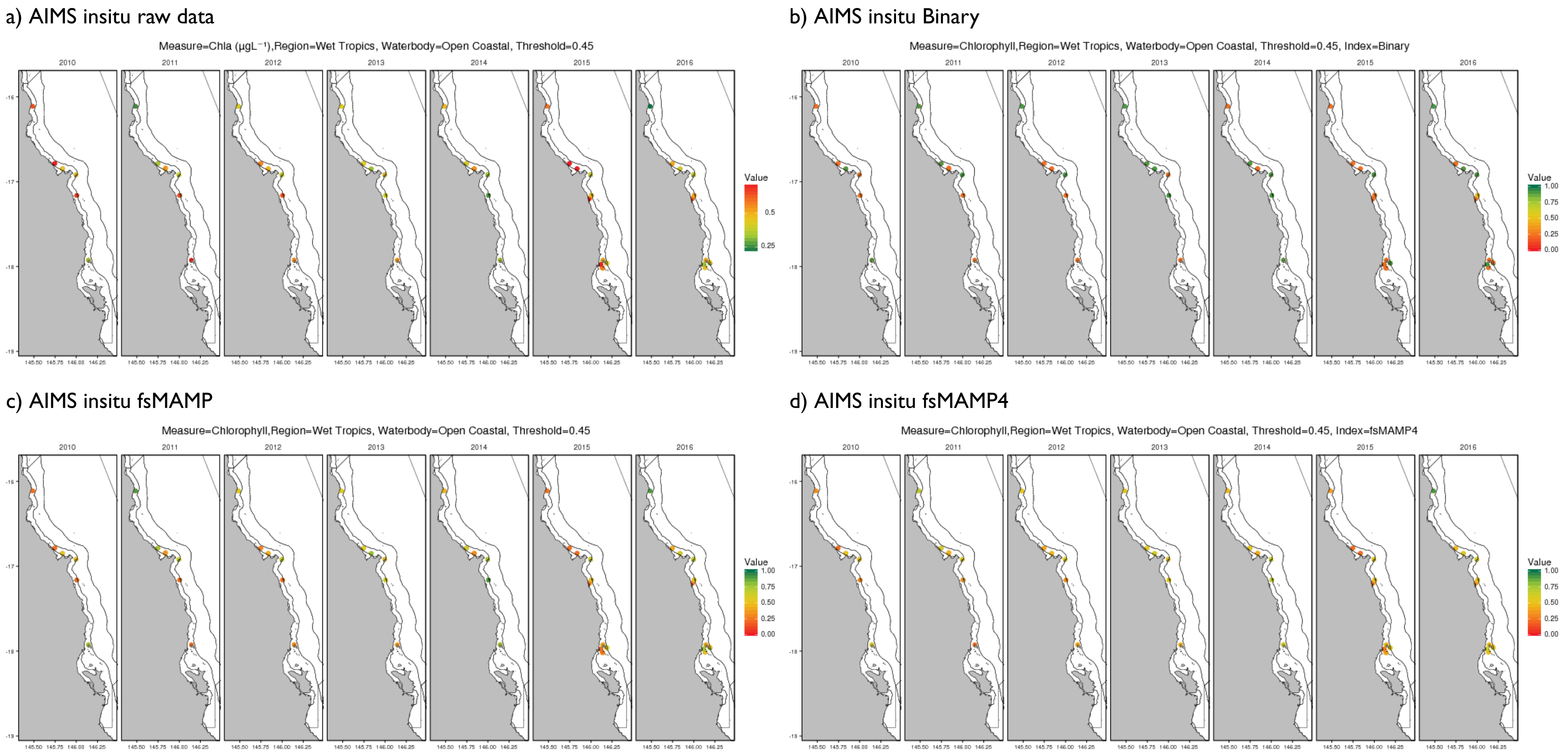


Figure 35: Spatial distribution of AIMS in situ Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

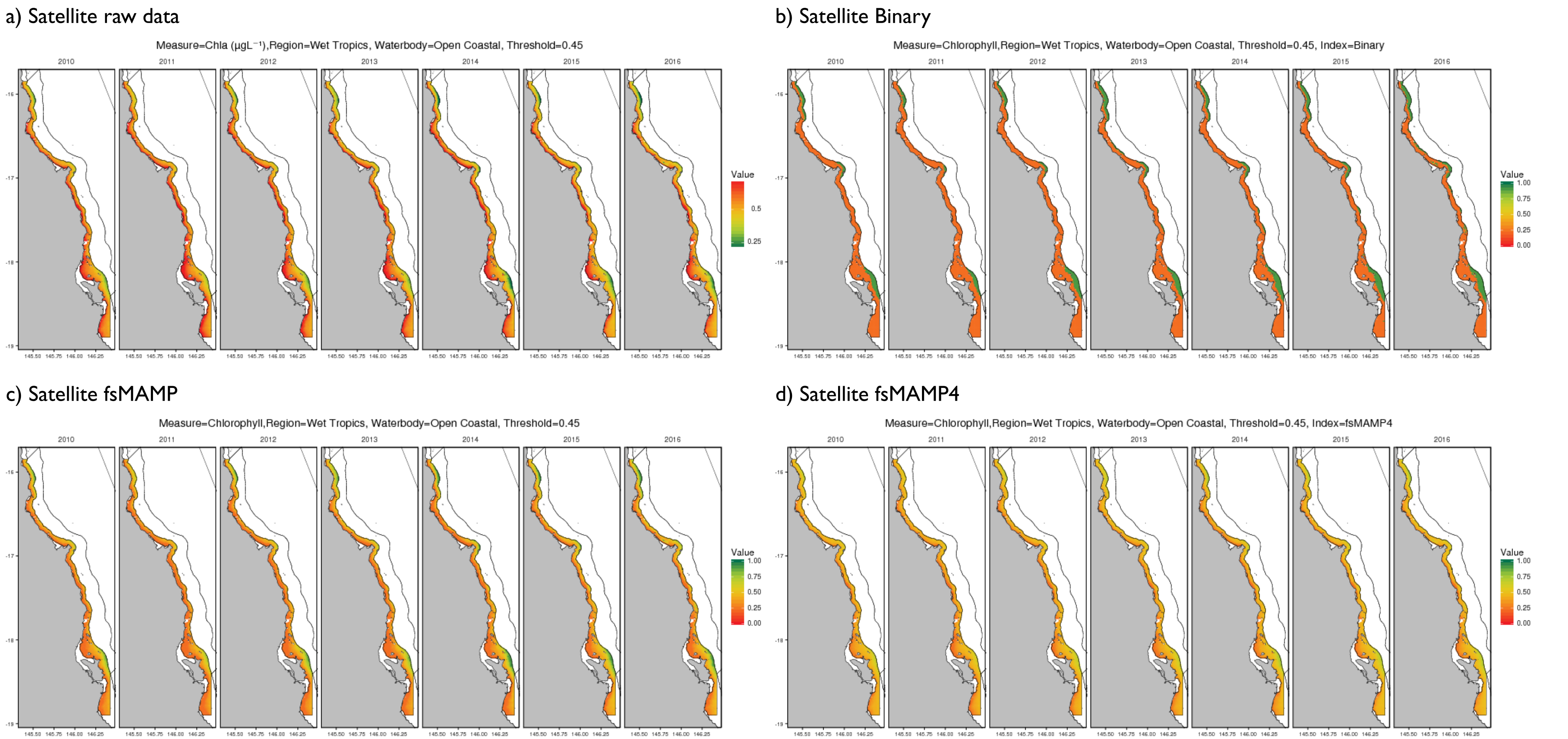


Figure 36: Spatial distribution of Satellite Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

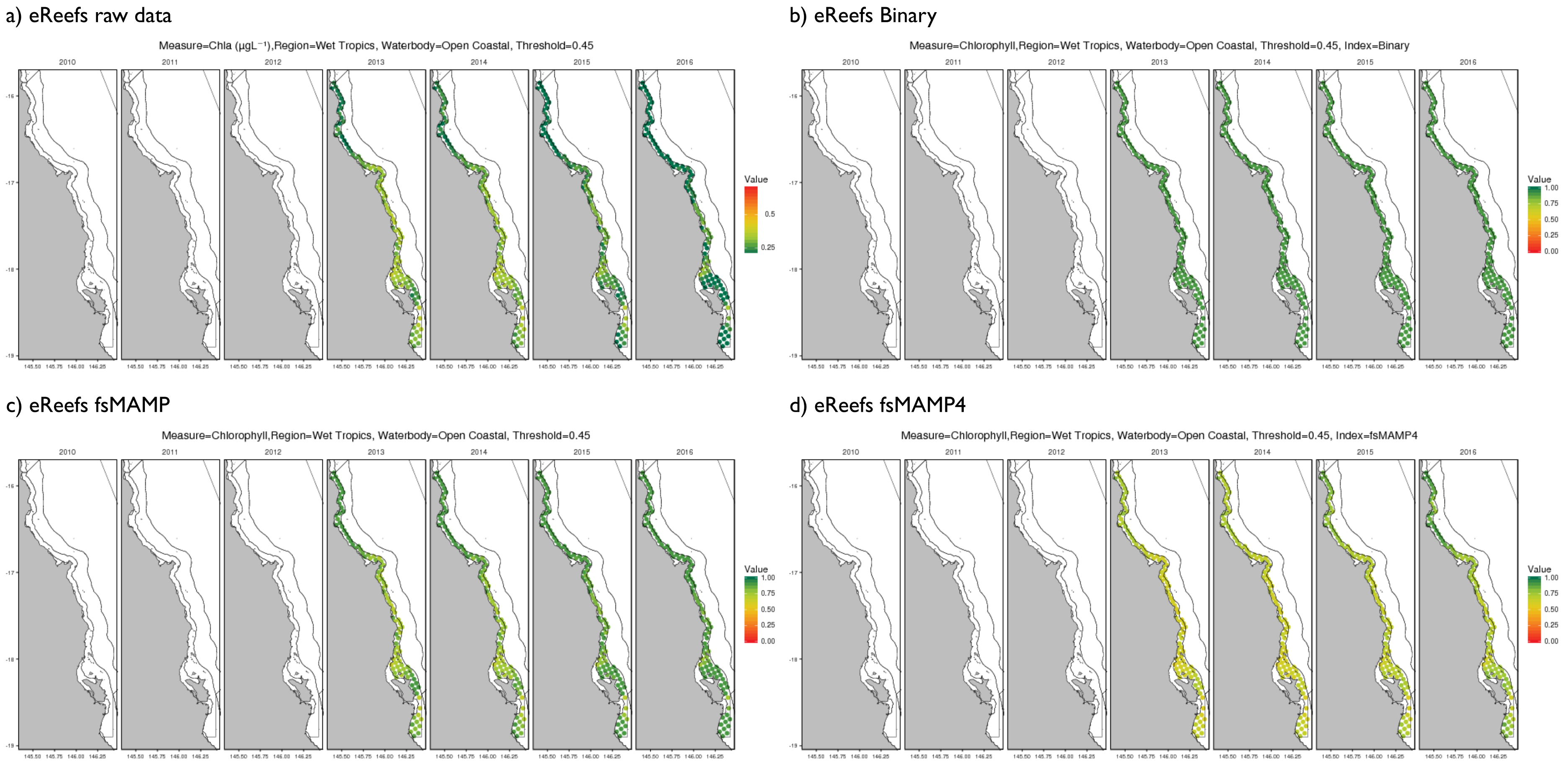


Figure 37: Spatial distribution of eReefs Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

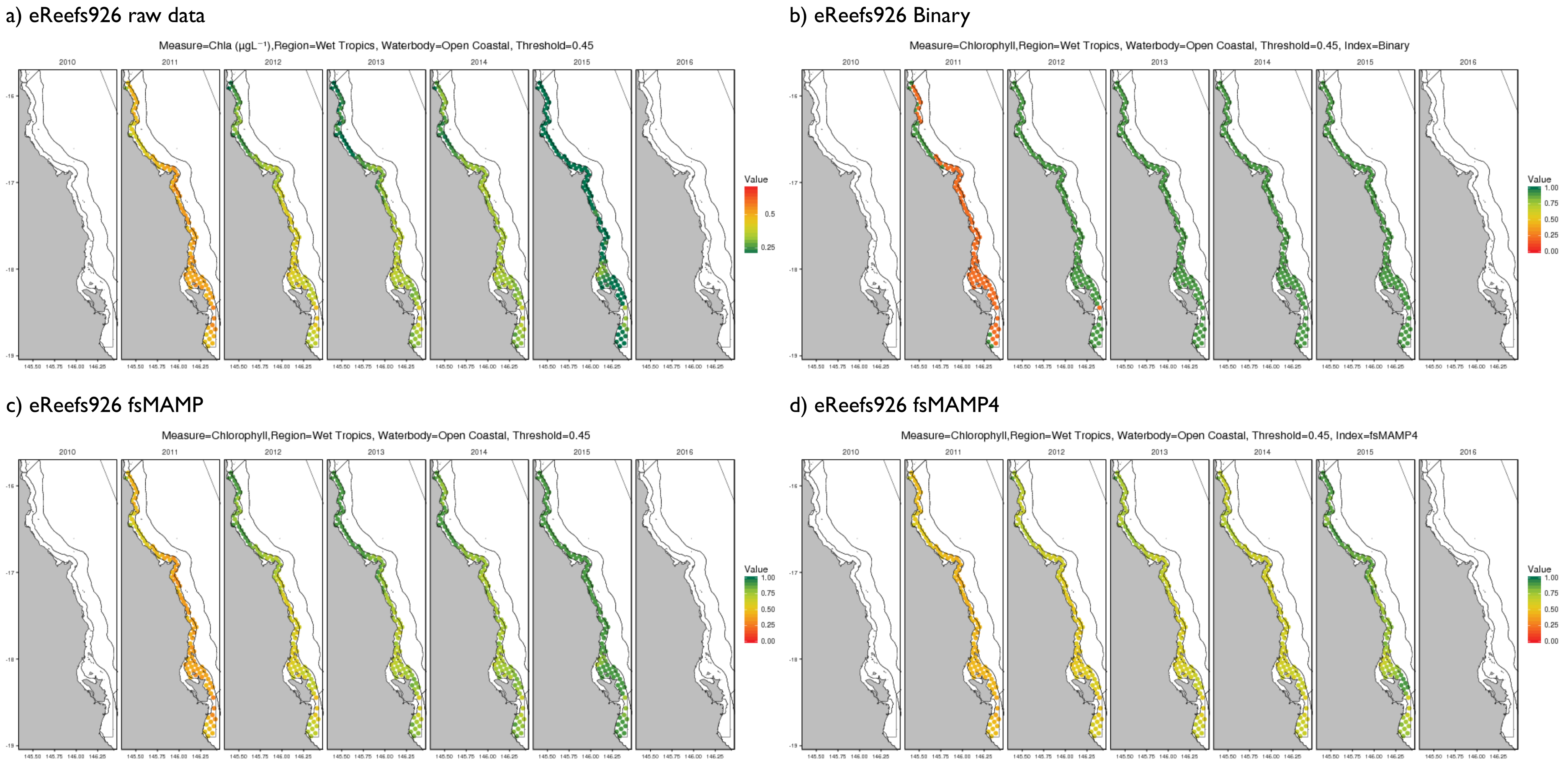
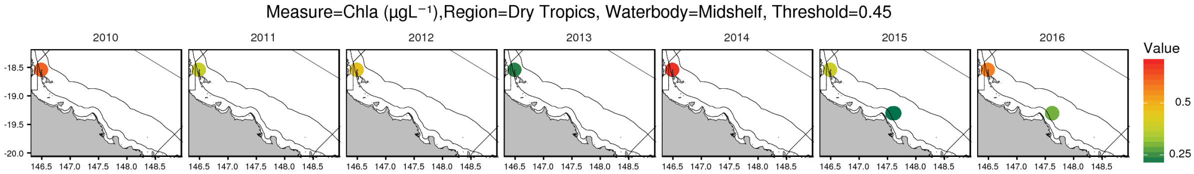
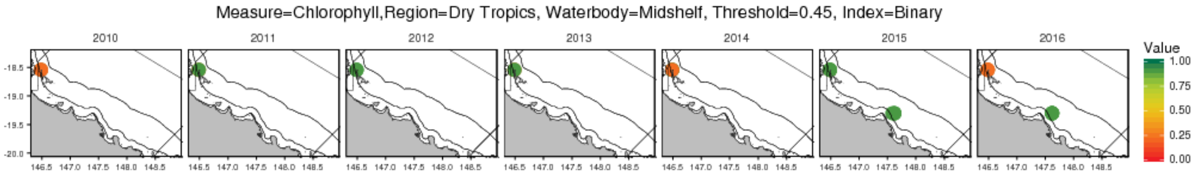


Figure 38: Spatial distribution of eReefs926 Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Wet Tropics Open Coastal zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

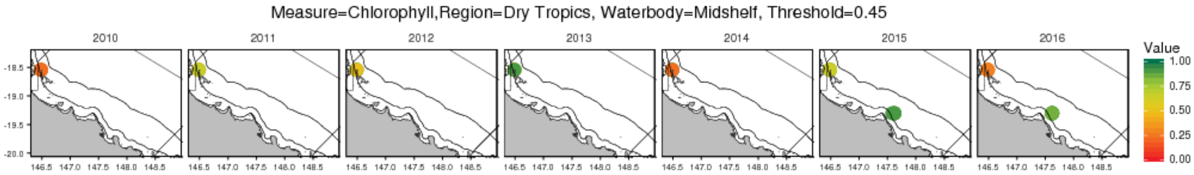
a) AIMS insitu raw data



b) AIMS insitu Binary



c) AIMS insitu fsMAMP



d) AIMS insitu fsMAMP4

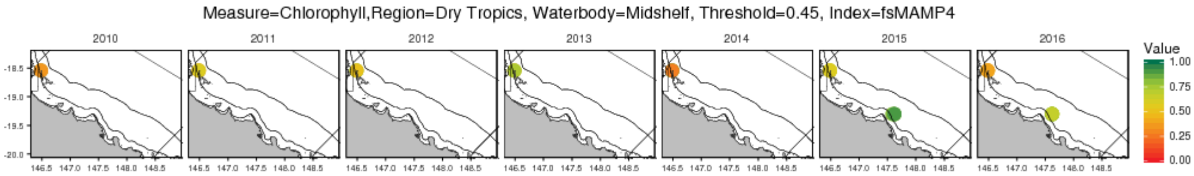
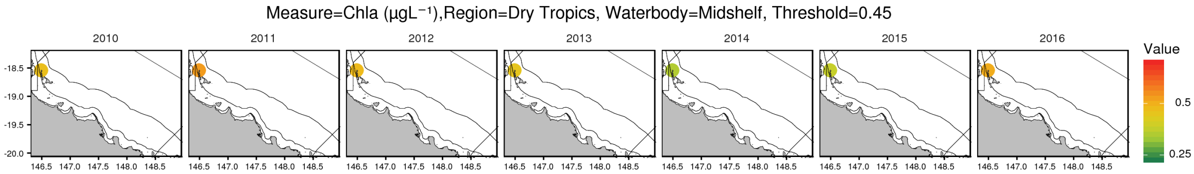
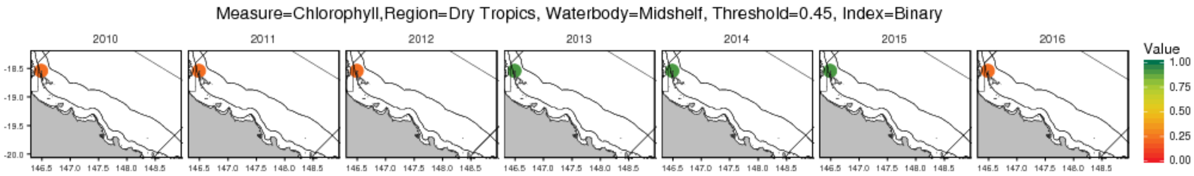


Figure 39: Spatial distribution of AIMS insitu Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Dry Tropics Midshelf zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

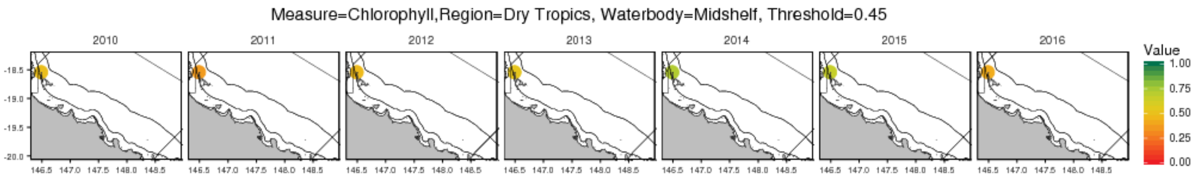
a) AIMS FLNTU raw data



b) AIMS FLNTU Binary



c) AIMS FLNTU fsMAMP



d) AIMS FLNTU fsMAMP4

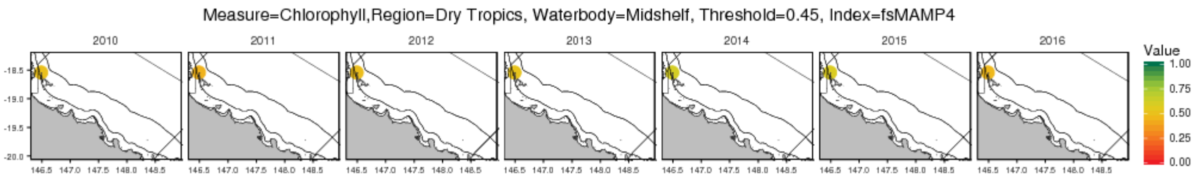
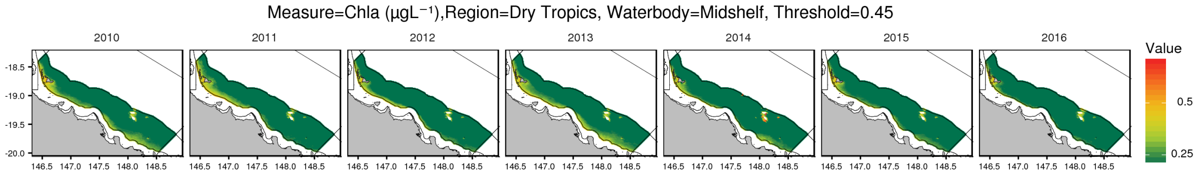
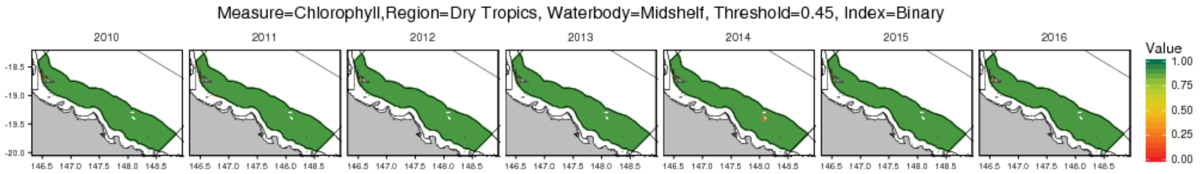


Figure 40: Spatial distribution of AIMS FLNTU Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Dry Tropics Midshelf zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

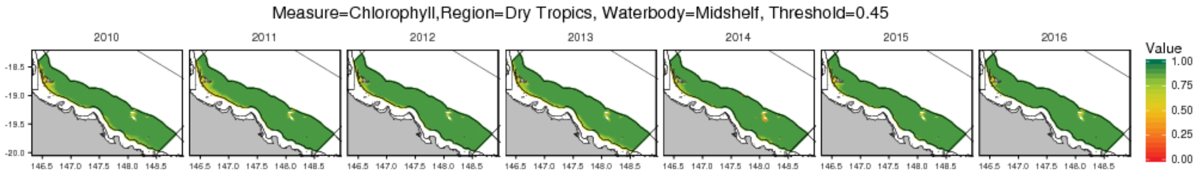
a) Satellite raw data



b) Satellite Binary



c) Satellite fsMAMP



d) Satellite fsMAMP4

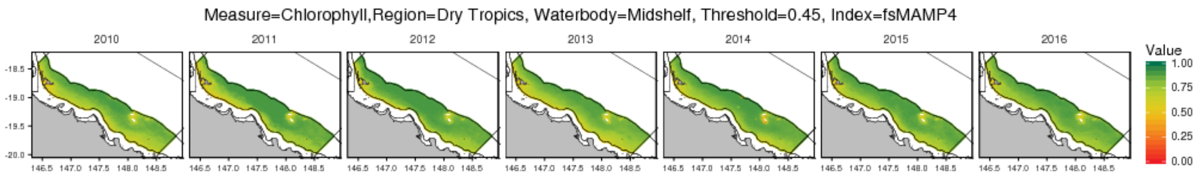
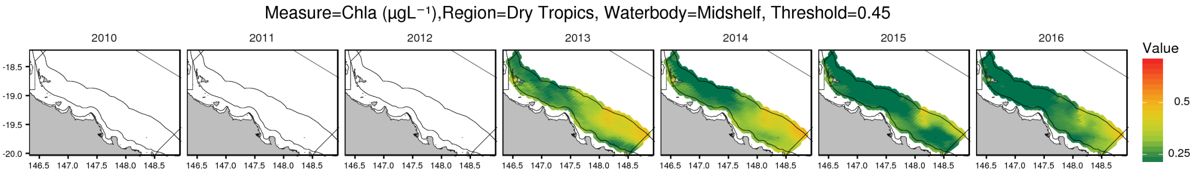
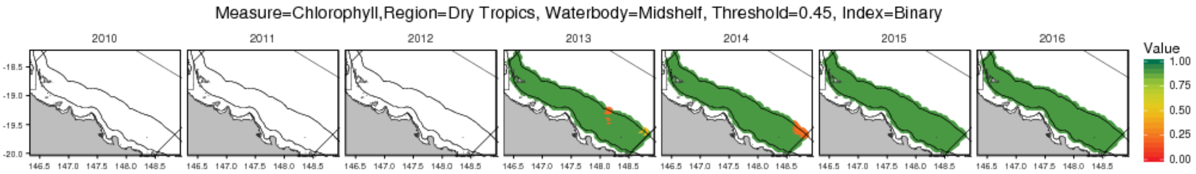


Figure 41: Spatial distribution of Satellite Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Dry Tropics Midshelf zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

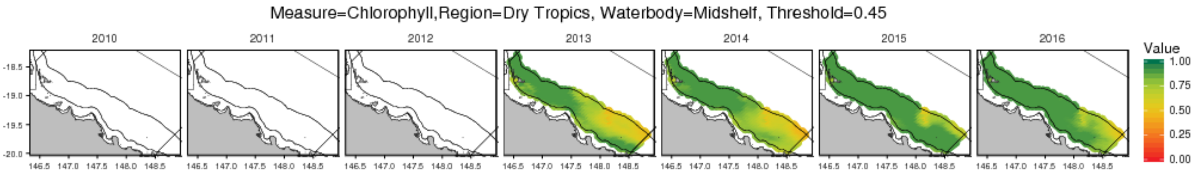
a) eReefs raw data



b) eReefs Binary



c) eReefs fsMAMP



d) eReefs fsMAMP4

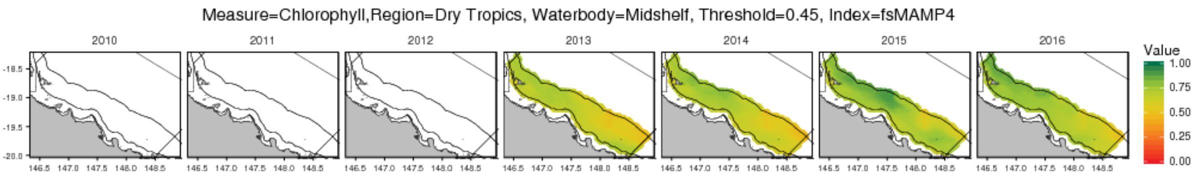
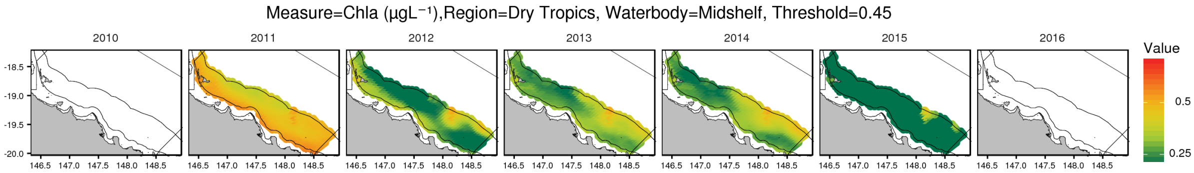
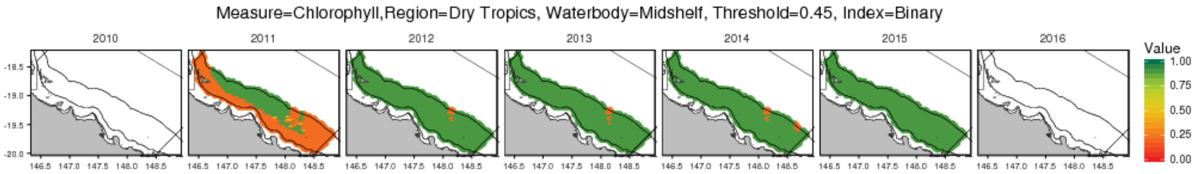


Figure 42: Spatial distribution of eReefs Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Dry Tropics Midshelf zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

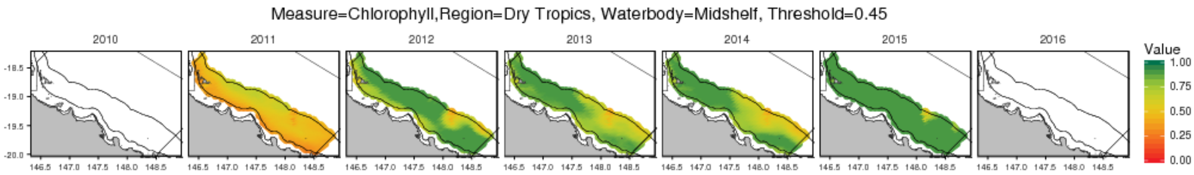
a) eReefs926 raw data



b) eReefs926 Binary



c) eReefs926 fsMAMP



d) eReefs926 fsMAMP4

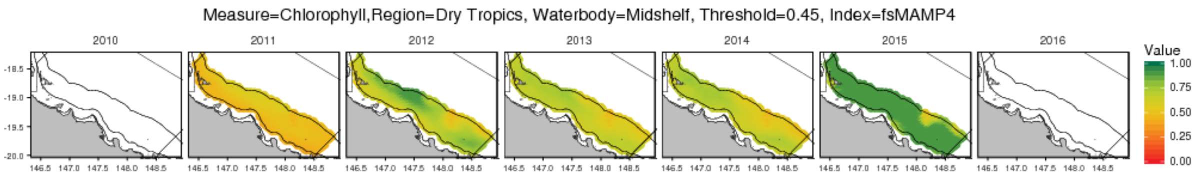


Figure 43: Spatial distribution of eReefs926 Chlorophyll-a a) samples and associated b) Binary, c) fsMAMP and d) fsMAMP4 index formulations for the Dry Tropics Midshelf zone. Color bars scaled to half (green) and twice (red) threshold value for raw data and 1 (green) and 0 (red) for Binary, fsMAMP and fsMAMP4.

Figure 44: Time series of annually aggregated Binary, fsMAMP and fsMAMP4 index formulations for AIMS insitu Chlorophyll-a across each of the Regions and Water bodies. The blue vertical bar spans from mid 2009 to mid 2011.

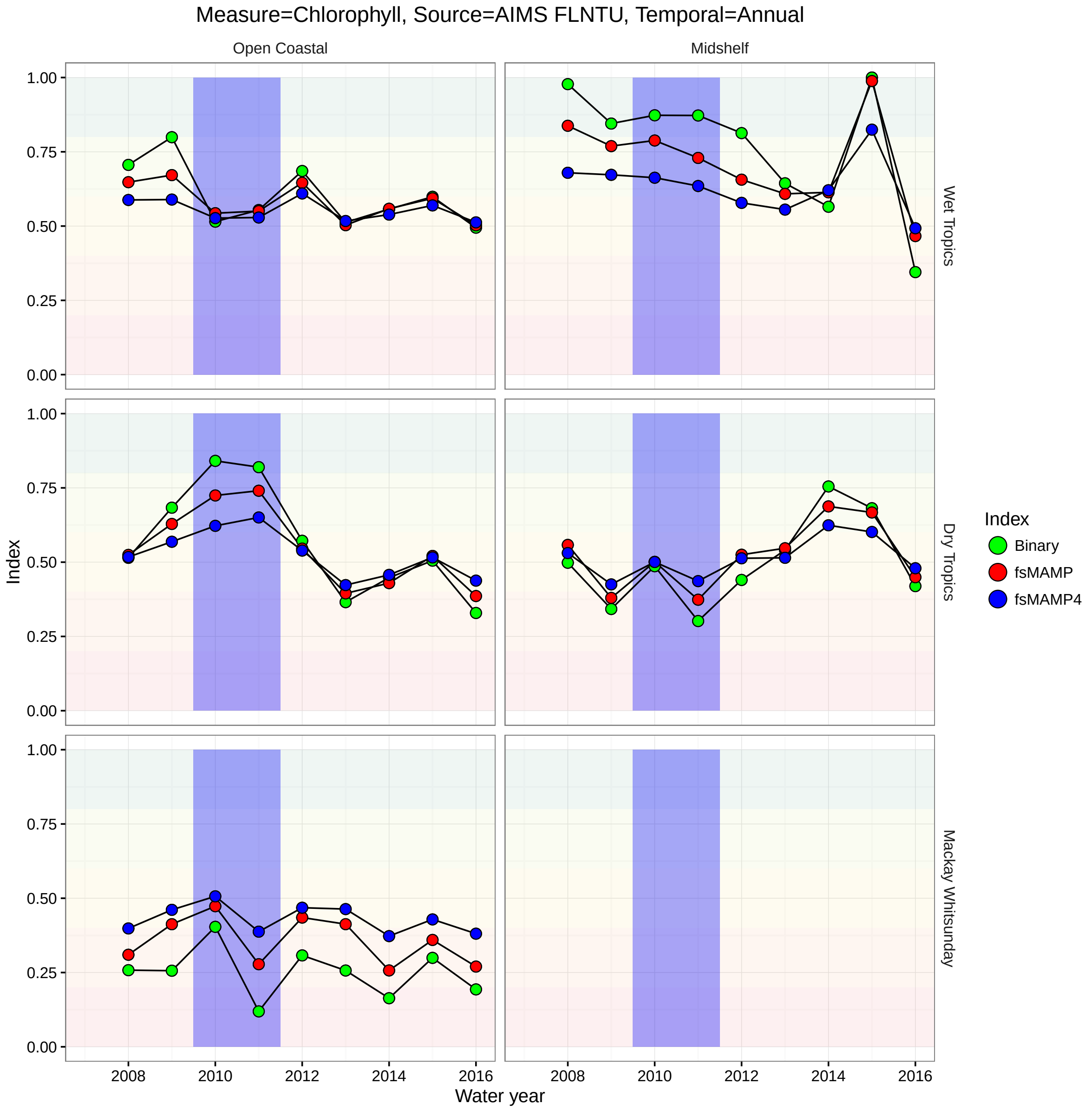


Figure 45: Time series of annually aggregated Binary, fsMAMP and fsMAMP4 index formulations for AIMS FLNTU Chlorophyll-a across each of the Regions and Water bodies. The blue vertical bar spans from mid 2009 to mid 2011.

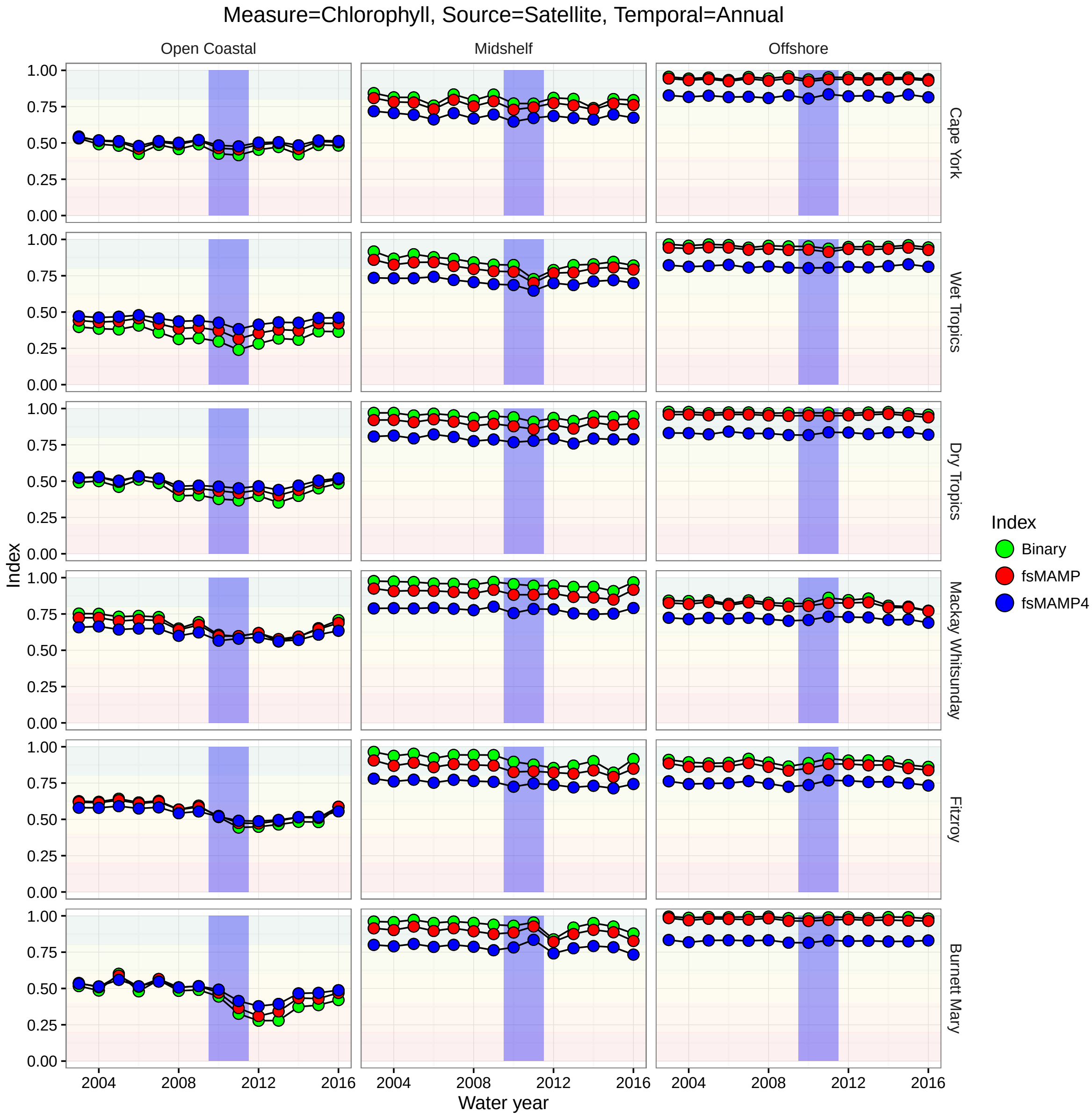


Figure 46: Time series of annually aggregated Binary, fsMAMP and fsMAMP4 index formulations for Satellite Chlorophyll-a across each of the Regions and Water bodies. The blue vertical bar spans from mid 2009 to mid 2011.

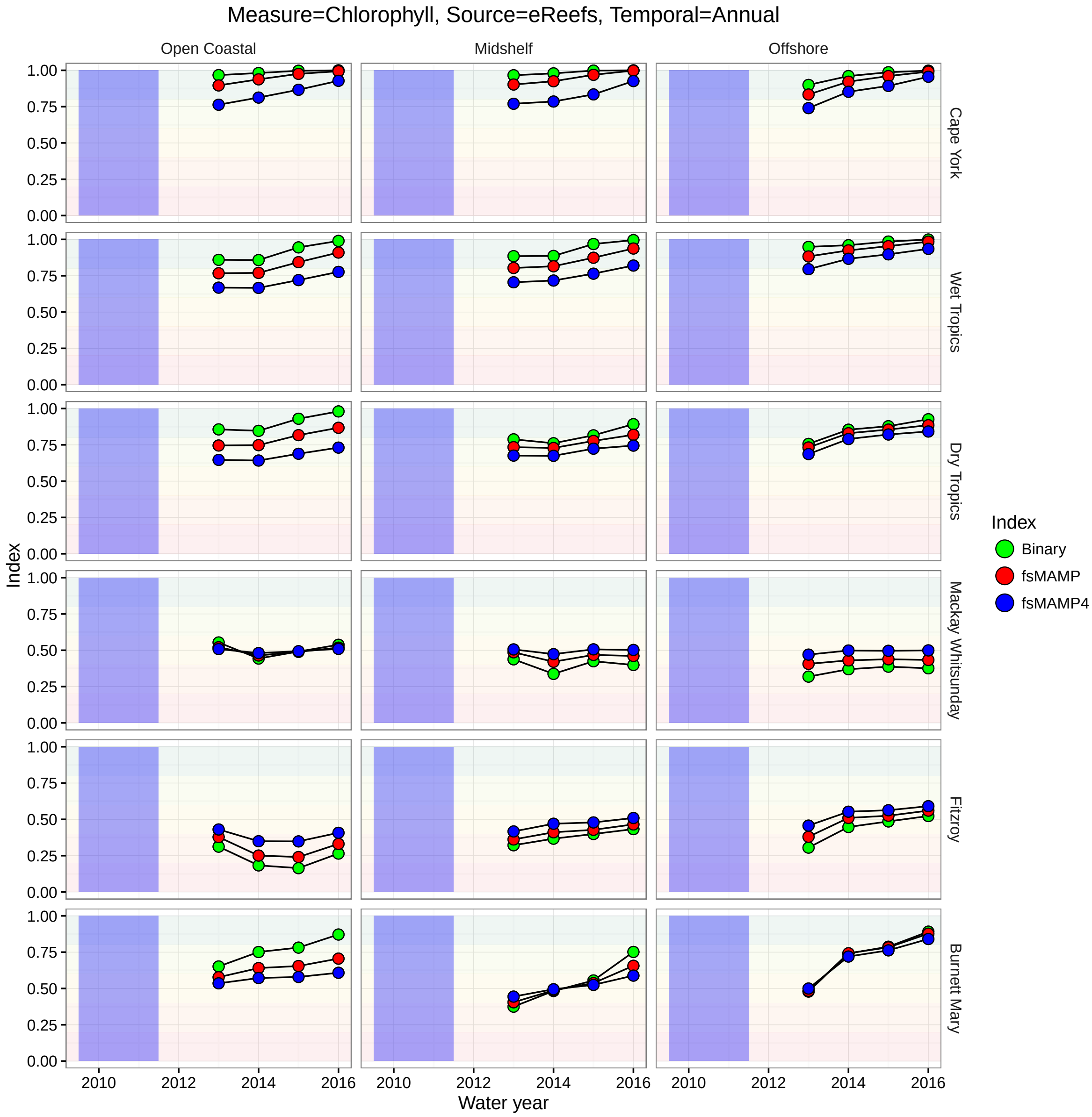


Figure 47: Time series of annually aggregated Binary, fsMAMP and fsMAMP4 index formulations for eReefs Chlorophyll-a across each of the Regions and Water bodies. The blue vertical bar spans from mid 2009 to mid 2011.

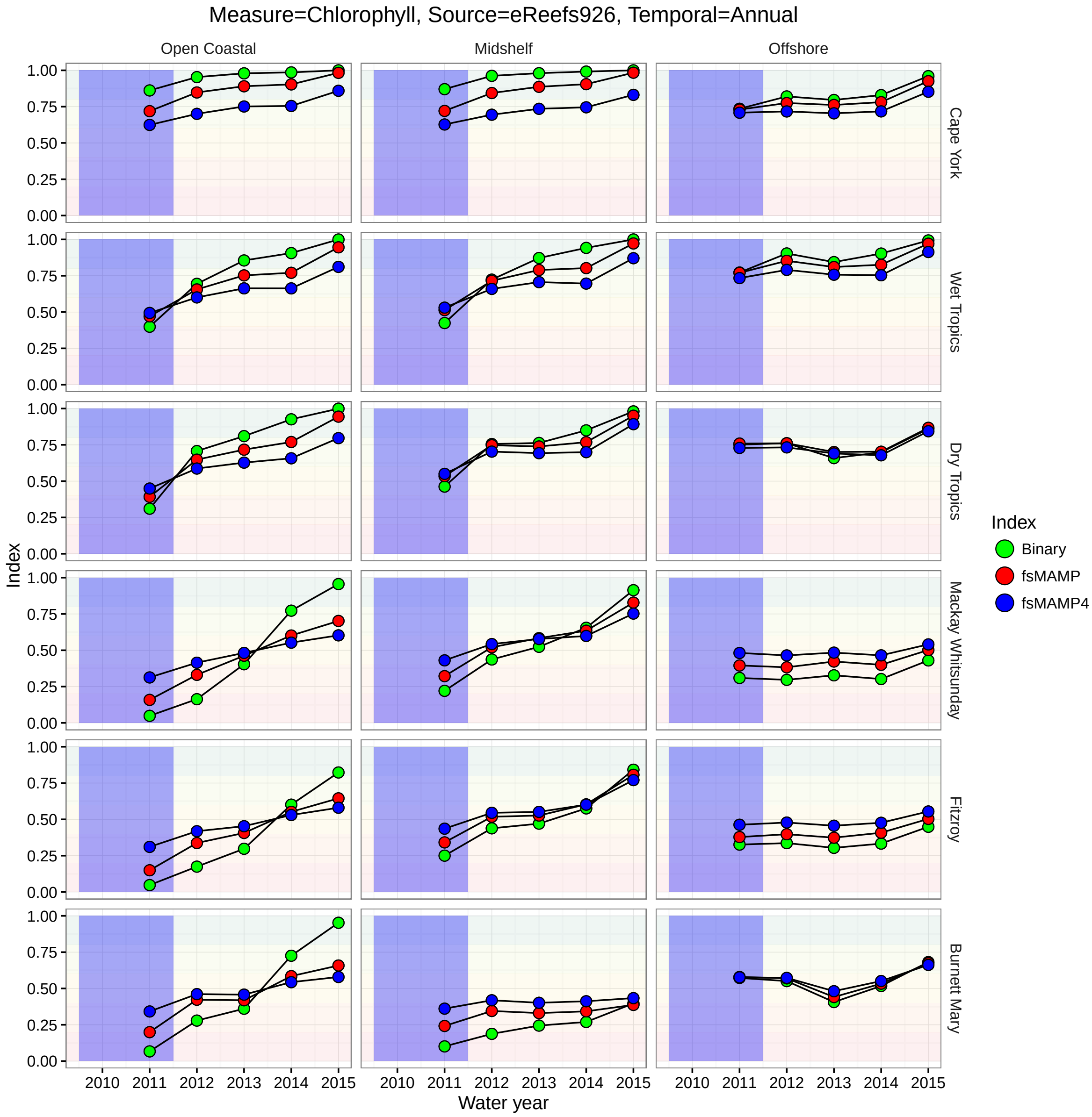


Figure 48: Time series of annually aggregated Binary, fsMAMP and fsMAMP4 index formulations for eReefs926 Chlorophyll-a across each of the Regions and Water bodies. The blue vertical bar spans from mid 2009 to mid 2011.

5.3.2 Sources

Typically, the major aspects of a property like water quality are not directly measurable. Properties such as productivity, water clarity, nutrients, pesticides etc encapsulate a set of underlying conditions and yet themselves are not directly measurable. Directly measurable properties (such as Chlorophyll-a, total suspended solids etc) thus act as proxies for the more broader properties. As directly measurable entities, many of these measures have long monitoring histories and there are at least some understanding of the ecological role of these measures.

A major advantage of remote sensing and modelling products in the context of environmental monitoring is that they provide substantially greater spatial and temporal coverage. However, the majority of the parameters yielded from these tools are algorithmic approximations of traditional measures. Consequently, in the context of water quality, they produce proxies of proxies.

The current project has access to a variety of sources of water quality monitoring data (see Section ??) ranging from sparse, yet vigorous direct in situ measurements (AIMS insitu) and temporally rich, spatially sparse AIMS FLNTU logger data through to spatio-temporally extensive, yet patchy remote sensing MODIS Satellite data and multiple versions of eReefs modelled data. These different sources of data are likely to provide estimates of the parameters that differ in both location (such as mean) as well as scale (variability).

Whilst it is beyond the scope of the current project to undertake a full evaluation of the accuracy, robustness and reliability of each of these sources, the indexed data permit us to explore and compare the spatio-temporal patterns of each data source. In particular, we can focus on sensitivity as suggested by variability in spatio-temporal patterns of indices of each data source and whether these patterns are consistent with expert expectations.

It is reasonable to expect that the AIMS insitu data would be the most accurate of all the sources, however it is also likely that these observations only represent conditions over a very restricted space and time. The AIMS insitu data are predominantly the limited spatial coverage of the AIMS insitu data that limits its utility as input into a water quality metric for the entire Great Barrier Reef.

A motivating inspiration for this project was the perceived insensitivity of the Satellite data source and aspirations to improve the sensitivity of the water quality metric as a whole. It was hoped that the introduction of eReefs modelled data would result in a metric that yields patterns that are more consistent with assumed trends.

Figures 49 – 52 contrast the broad spatial and temporal patterns in aggregated fsMAMP Chlorophyll-a, TSS, Secchi depth and NOx indices. Within a zone (Region/Water body), the Satellite data (Remote sensing) are substantially less varied than the other sources. Obvious deviations in trajectory are only really apparent for the Open Coastal areas (although not for Cape York). Moreover, while the Satellite indices are suggestive of a cross-shelf (West to East) increase in water quality, this mainly occurs between Open Coastal and Midshelf and there is little (if any) consistent South-North water quality increase.

The AIMS insitu data result in the most sensitive metrics. However, the temporal deviances in data (and thus indices) could be exaggerated by the the proximal location of AIMS insitu sites relative to sources of major river discharge. Thus, this sensitivity could be artificially inflated and is unlikely to be unrepresentative. Moreover, the AIMS insitu data are restricted to just a subset (5/18) of the zones of interest.

Surprisingly, there is relatively little correspondence in trajectories between AIMS insitu and AIMS FLNTU logger data. These differences could be due either to differences in sampling designs (AIMS insitu have additional sites and thus represent a different spatial domains, AIMS FLNTU have substantially greater temporal coverage and thus are potentially more representative over time) and could also reflect direct (AIMS insitu) vs indirect (AIMS FLNTU) nature of the measurements. Either way, it is difficult endorse either of these sources as a primary data source on which to construct GBR wide Water Quality metrics.

The broad spatial pattern of both eReefs and eReefs926 appear to follow the overall expectations of South - North and West - East gradients[10], with Chlorophyll-a typically increasing from S to N and W to E - more so for eReefs926 than eReefs. Unfortunately it is difficult to assess the sensitivity of temporal patterns in eReefs and eReefs926 data sources due to their relatively short availability windows. In particular, it is inconvenient that neither eReefs source extend back to the 2010–2011 wet years to provide some form of qualitative calibration.

Underlying alterations in the eReefs biogeochemical model have resulted in some relatively large changes for each of Chlorophyll-a, Secchi depth and NOx and evaluating the causes of these differences is beyond the scope of the current study

[10]less obvious for TSS and NOx

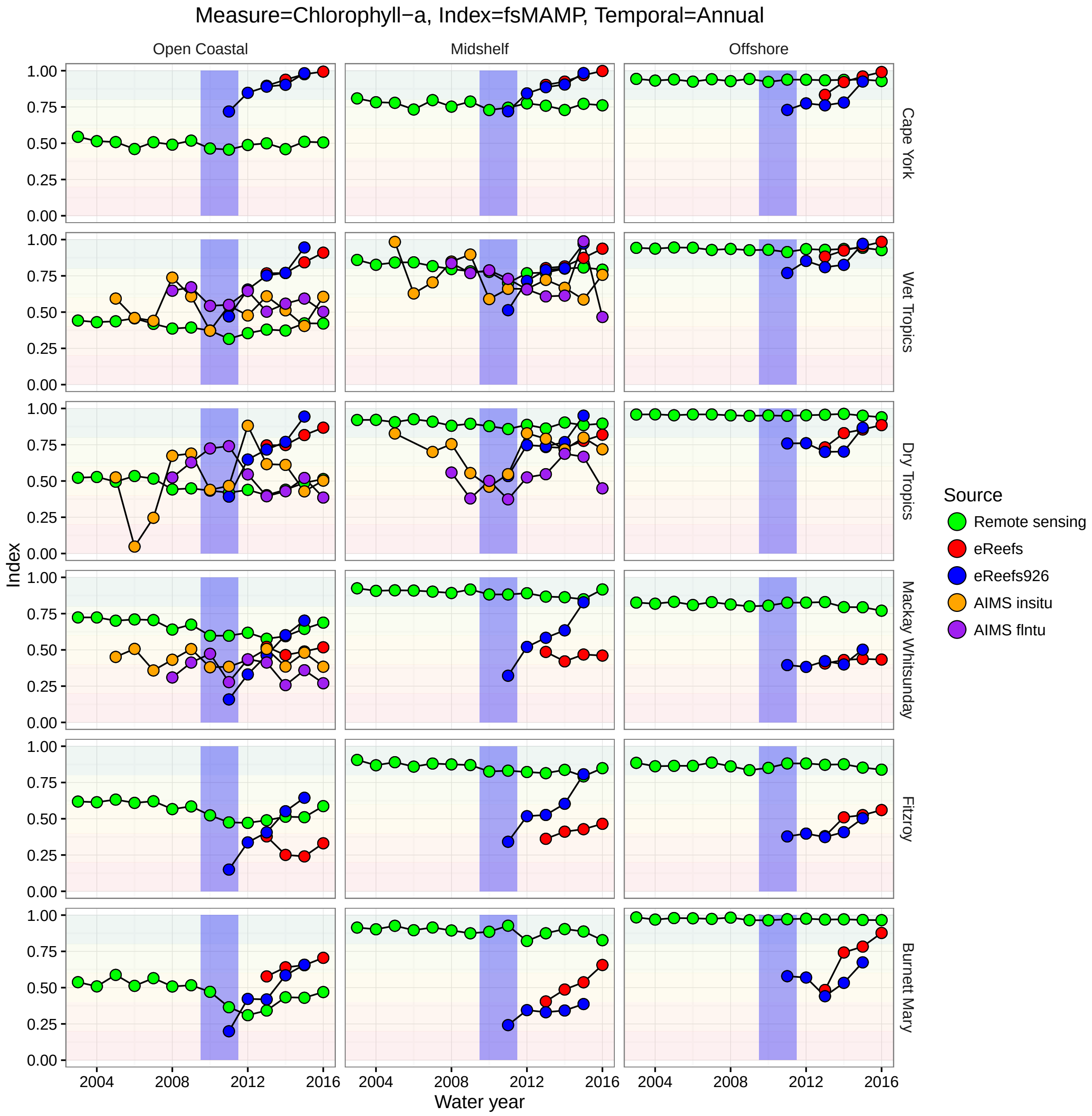


Figure 49: Time series of fsMAMP Chlorophyll-a index scores by zone for each data source. The blue vertical bar spans from mid 2009 to mid 2011.

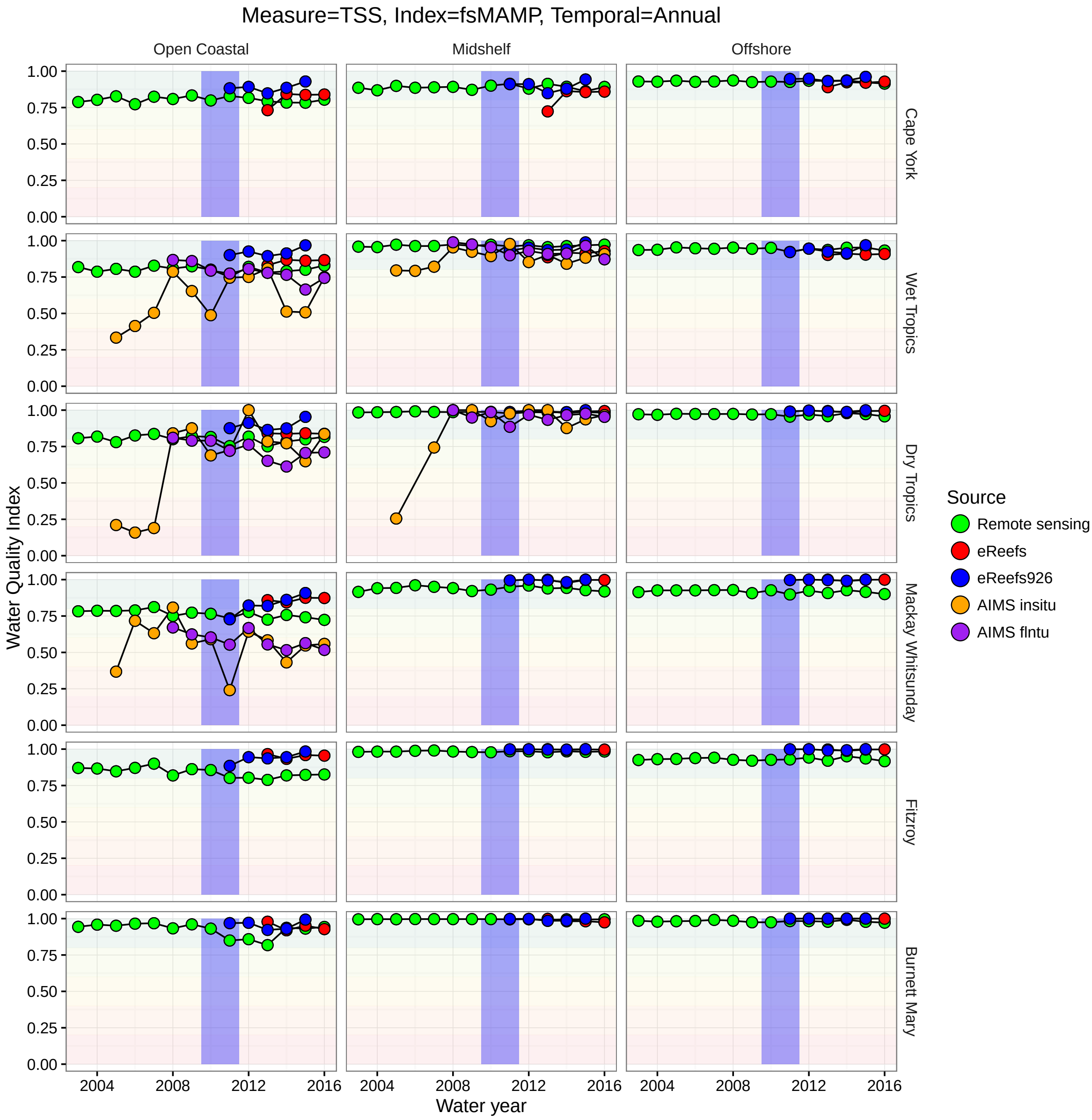


Figure 50: Time series of fsMAMP TSS index scores by zone for each data source. The blue vertical bar spans from mid 2009 to mid 2011.

Figure 51: Time series of fsMAMP Secchi depth index scores by zone for each data source. The blue vertical bar spans from mid 2009 to mid 2011.

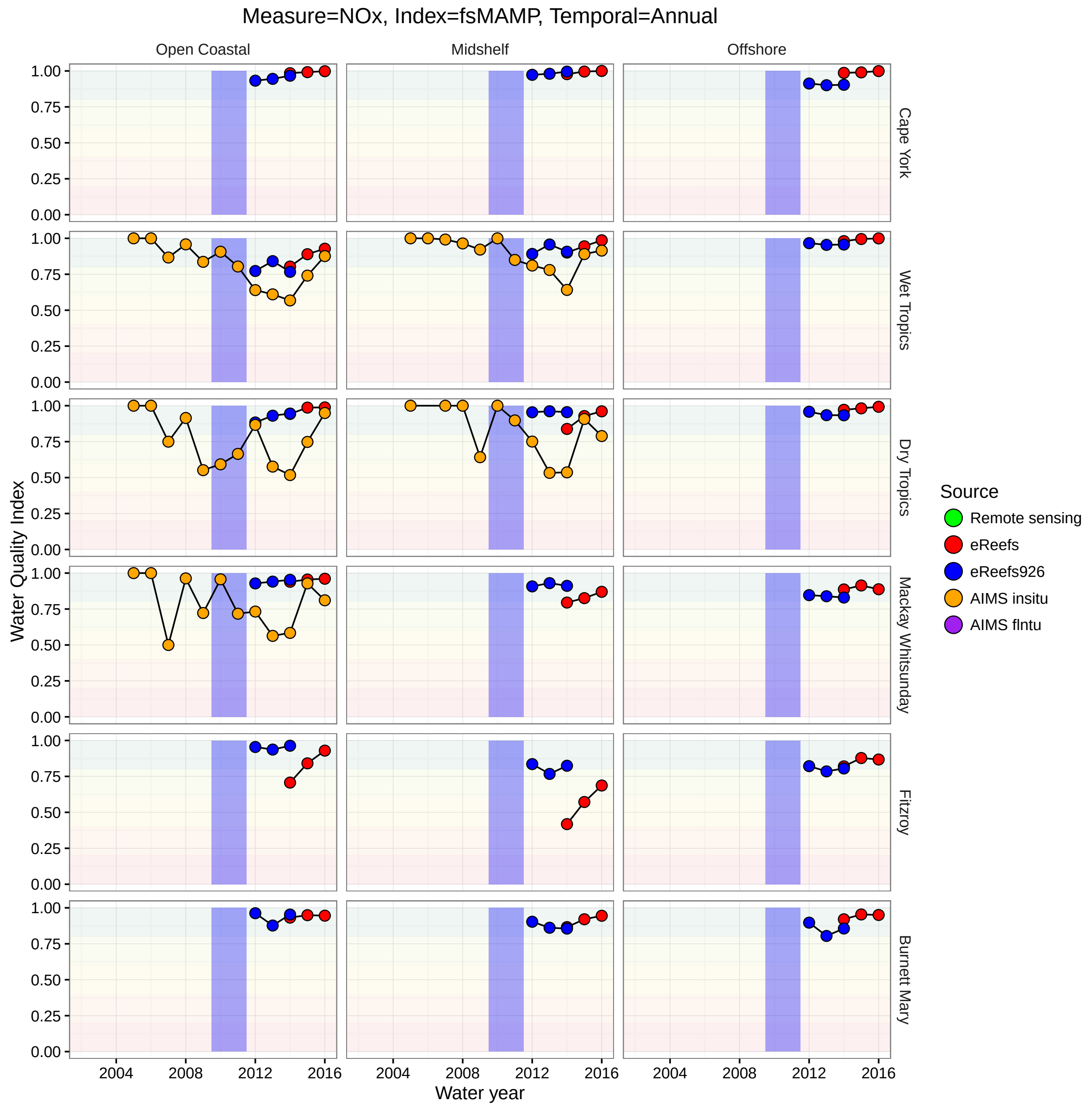


Figure 52: Time series of fsMAMP NOx index scores by zone for each data source. The blue vertical bar spans from mid 2009 to mid 2011.

5.3.3 Exploration of Measures

A Water Quality Index should attempt to reflect multiple properties of the underlying water bodies. For example, Water Quality could be characterized by combinations of Productivity, Water clarity, Nutrients, Toxicants etc. In turn, each of the above Sub-indicators, can be characterized by actual measureable properties (such as Chlorophyll-a, Total Suspended Solids, Total Nitrogen etc).

Typically, a Water Quality index is limited to what measureable properties are available and have appropriate guidelines (thresholds). The spatial extent of the current application of Water Quality metrics limits the Measures to Chlorophyll-a, Total Suspended Solids, Secchi Depth and NOx (Nitrite + Nitrate). Temporal series of the individual Measures for each Zone (based on fsMAMP of eReefs data) are presented in Figure 53.

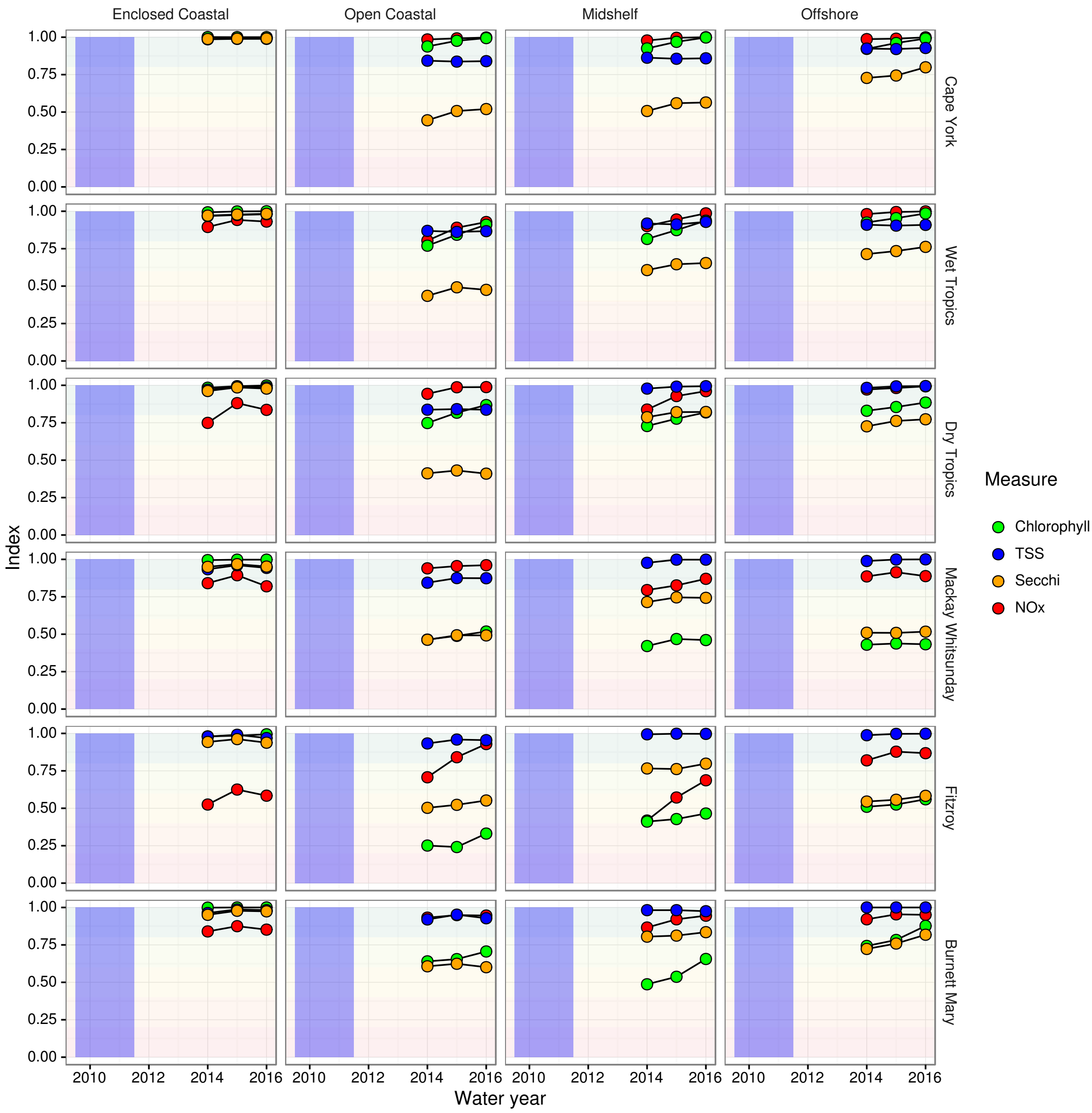


Figure 53: Time series of fsMAMP NOx index scores by zone for each data source. The blue vertical bar spans from mid 2009 to mid 2011.

These four Measures can be placed in a aggregation hierarchy such as depicted in Table 7.

Table 7: Hierarchical association between Measures, Sub-indicators and Indicators.

Measure	Sub-indicator	Indicator
Chlorophyll-a	Productivity	Water Quality
Total Suspended Solids	Water Clarity	Water Quality
Secchi Depth	Water Clarity	Water Quality
NOx	Nutrients	Water Quality

Nevertheless, the reliability and utility of each of these Measures are not necessarily equal. A number of candidate Measure combinations[11] are considered (see below). The contributions of each Measure to the corresponding Water Quality Indicator Scores (based on the hierarchy presented in Table 7) are:

- Chlorophyll-a $(1/3)$, TSS $(1/2 \times 1/3 = 1/6)$, SD $(1/2 \times 1/3 = 1/6)$ and NOx $(1/3)$
- Chlorophyll-a $(1/3)$, TSS $(1/2 \times 1/2 = 1/4)$, SD $(1/2 \times 1/2 = 1/4)$
- Chlorophyll-a $(1/2)$, SD $(1/2)$
- Chlorophyll-a $(1/2)$, TSS $(1/2)$

For each candidates, eReefs data with fsMAMP formulations will be presented (see Figure 54).

Figure 54: Time series of eReefs fsMAMP Measure Index Scores by zone. The blue vertical bar spans from mid 2009 to mid 2011.

Water Quality Indicator Scores based on candidate combinations that include either Chl, TSS, SD and NOx or Chl and TSS are considered very similar. Water Quality Indicator Scores are substantially lowered by the inclusion of Secchi Depth, the severity of which depends on the degree of dilution by other Measures.

[11] These effectively act as weights

5.3.4 Measure/Site

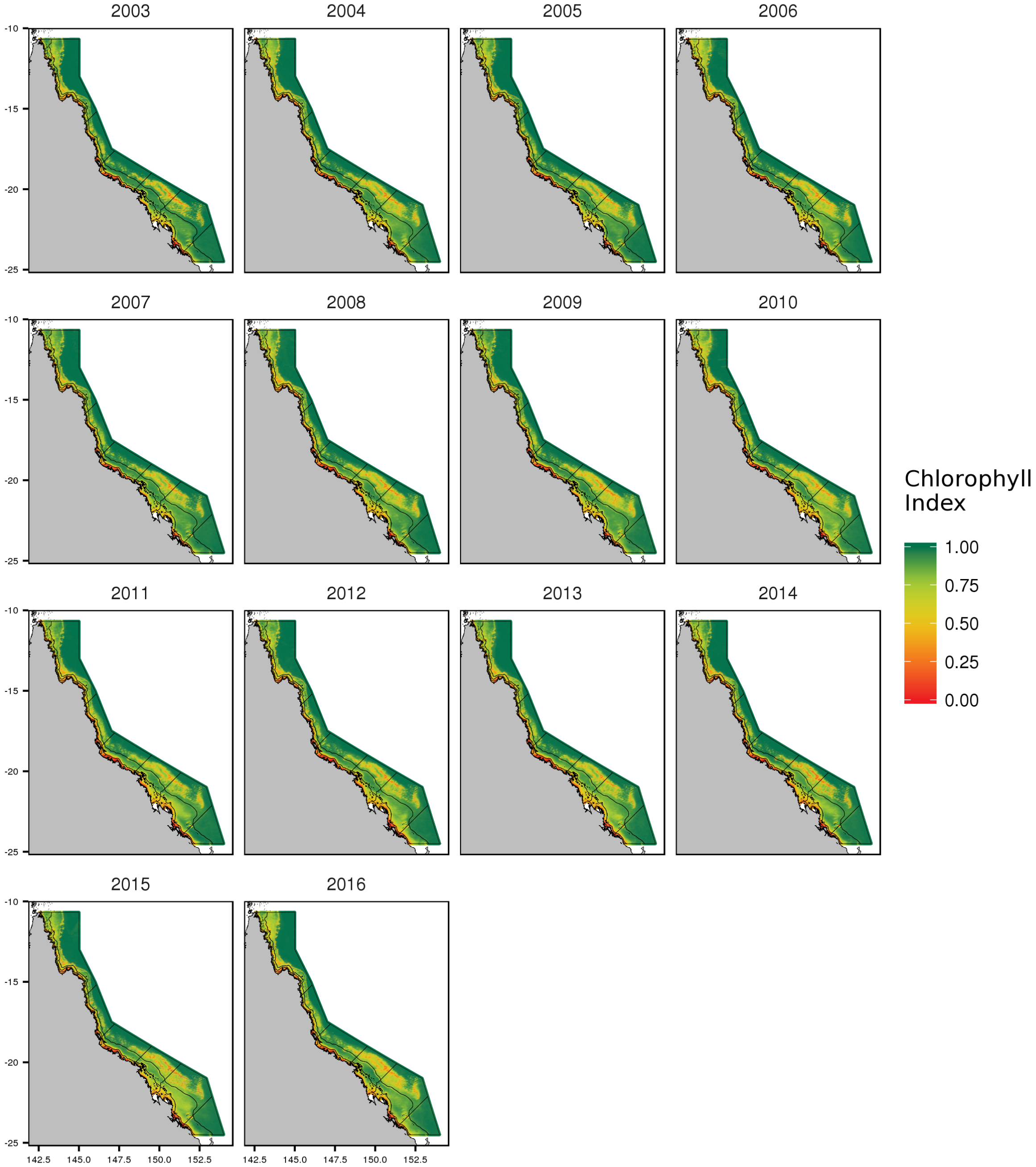


Figure 55: Spatio-temporal Satellite fsMAMP Chlorophyll-a index scores.

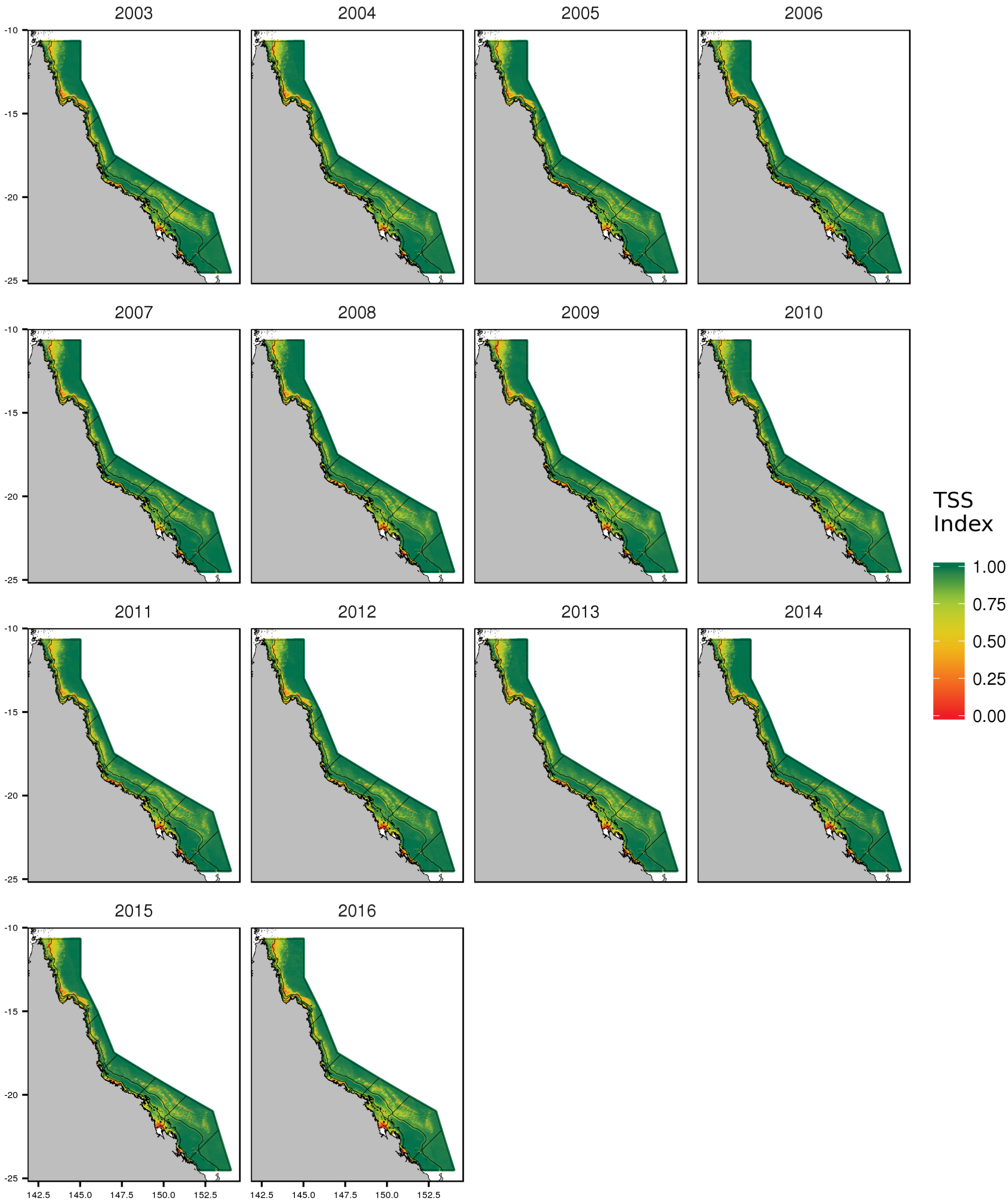


Figure 56: Spatio-temporal Satellite fsMAMP TSS index scores.

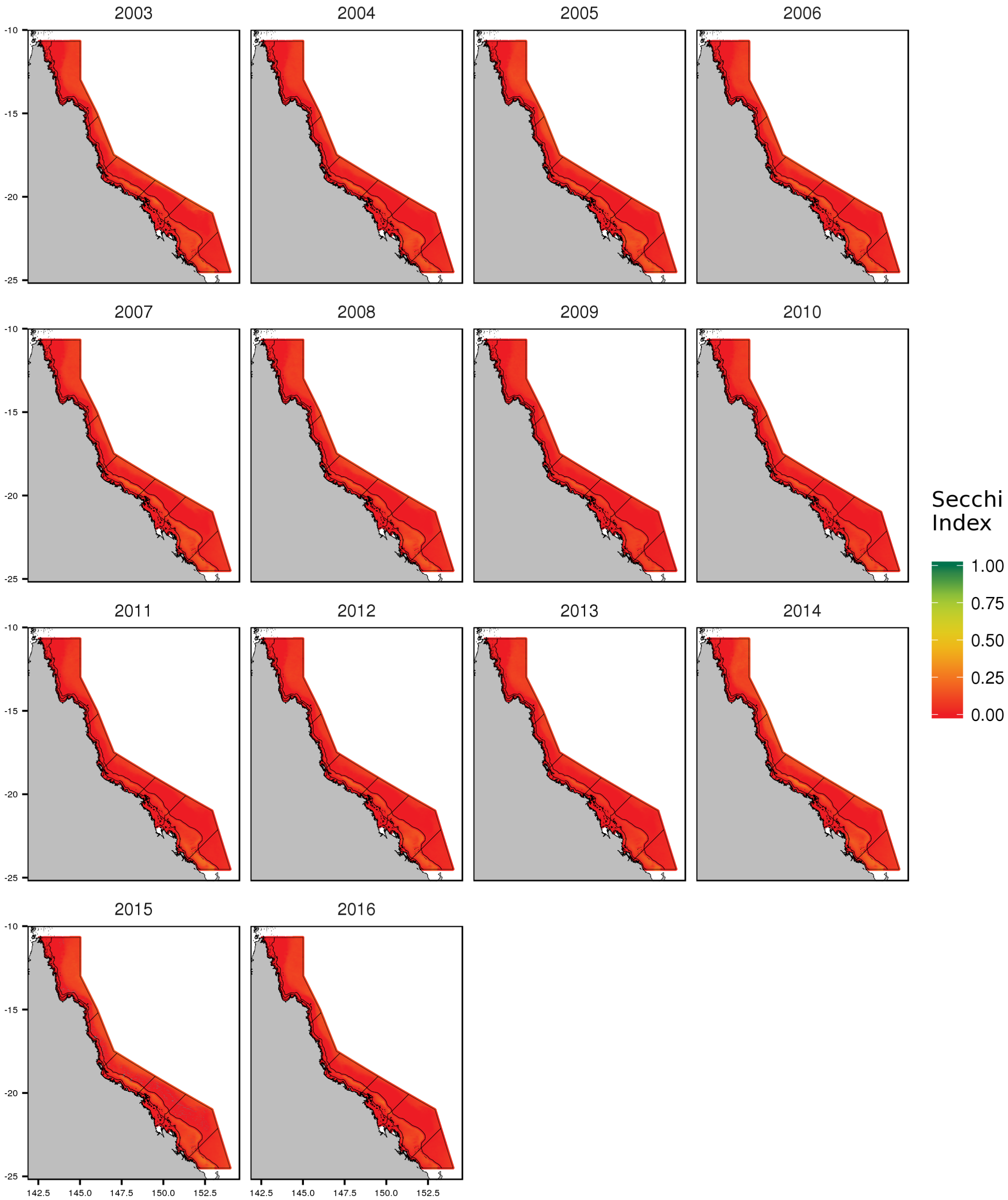


Figure 57: Spatio-temporal Satellite fsMAMP Secchi depth index scores.

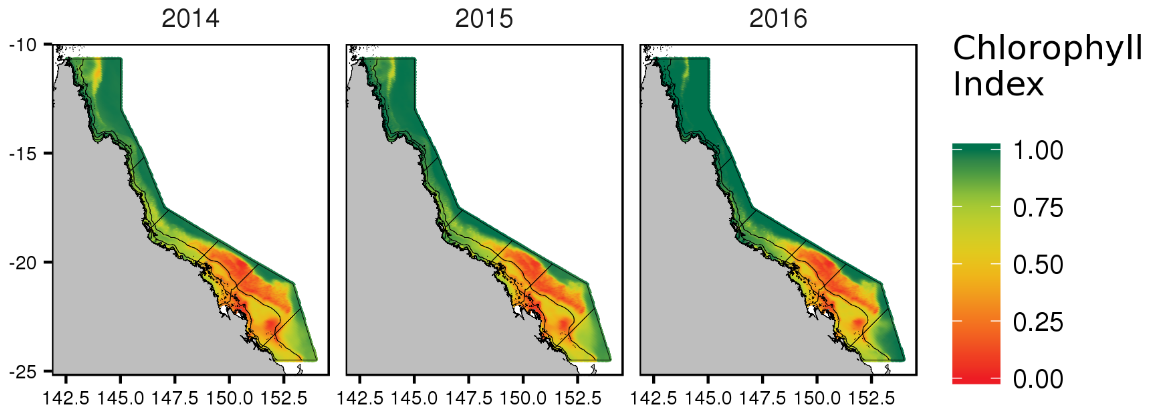


Figure 58: Spatio-temporal eReefs fsMAMP Chlorophyll-a index scores.

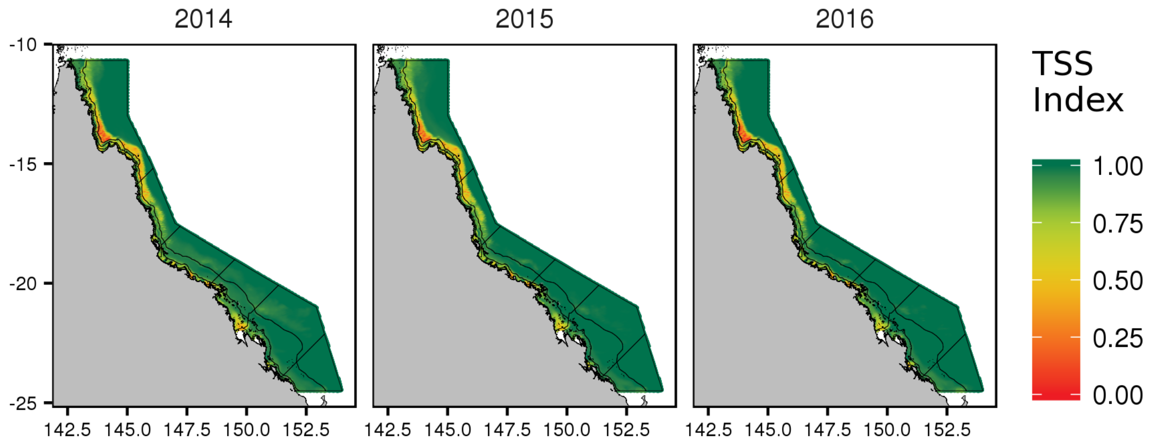


Figure 59: Spatio-temporal eReefs fsMAMP TSS index scores.

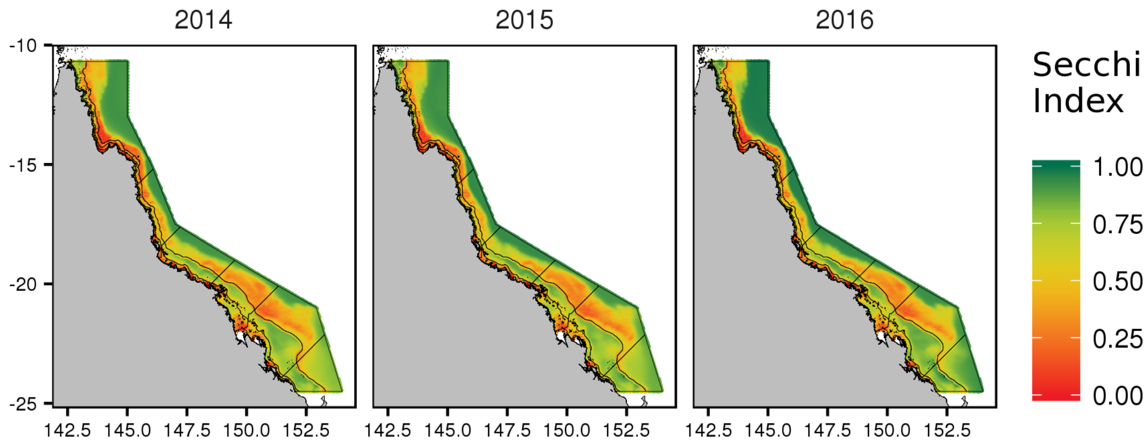


Figure 60: Spatio-temporal eReefs fsMAMP Secchi depth index scores.

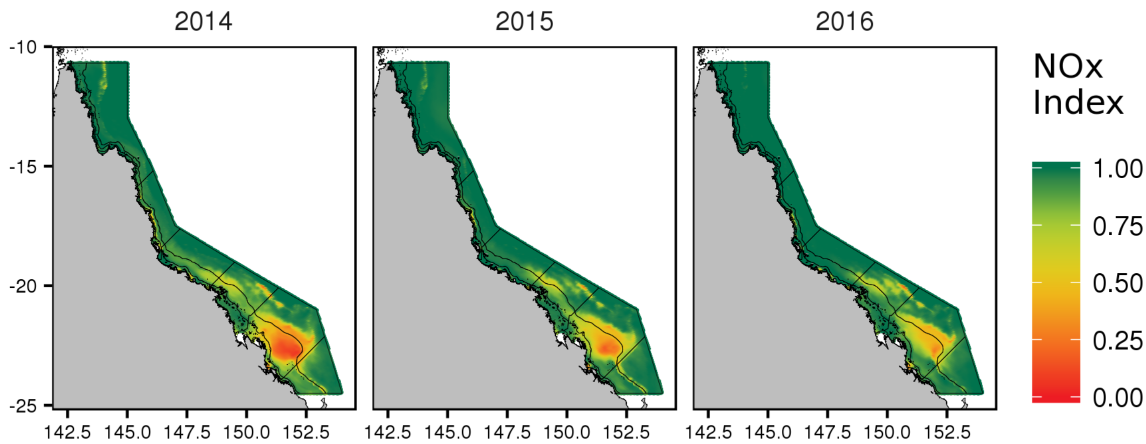


Figure 61: Spatio-temporal eReefs fsMAMP NOx index scores.

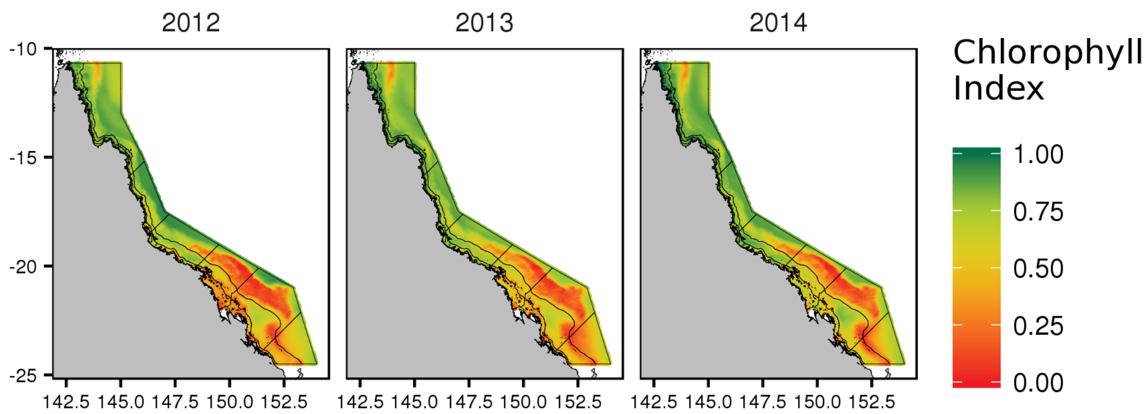


Figure 62: Spatio-temporal eReefs926 fsMAMP Chlorophyll-a index scores.

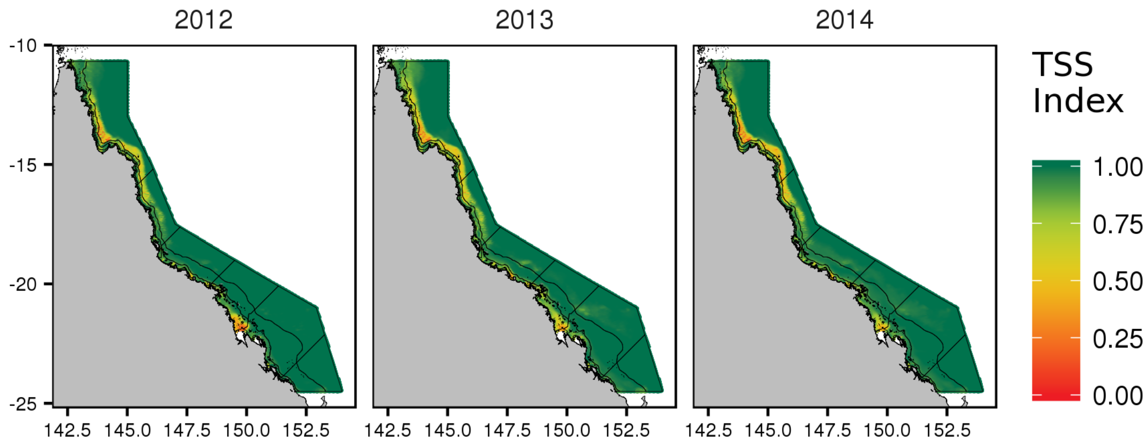


Figure 63: Spatio-temporal eReefs926 fsMAMP TSS index scores.

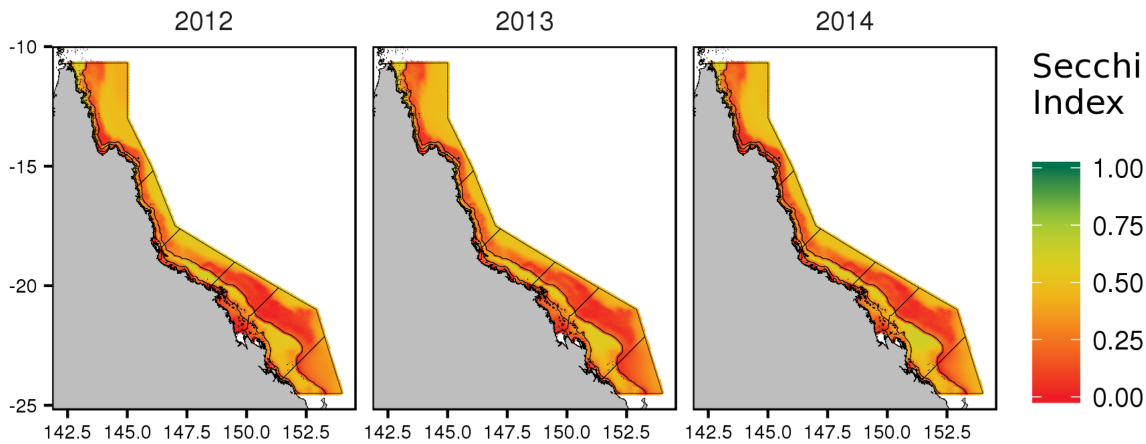


Figure 64: Spatio-temporal eReefs926 fsMAMP Secchi depth index scores.

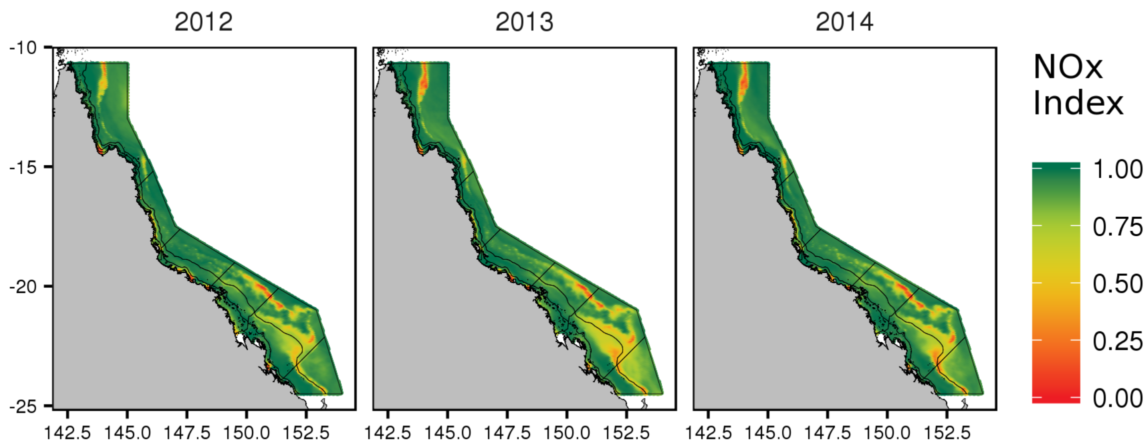


Figure 65: Spatio-temporal eReefs926 fsMAMP NOx index scores.

5.4 Summary of recommendations

6. HIERARCHICAL AGGREGATIONS

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Appendicies

A. THRESHOLDS

B. EREEFS MODELS

C. EXPLORATORY DATA ANALYSIS