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Kristin Jacobs Coral Reef Ecosystem Conservation Area Water Quality Assessment: Part 2

Final Report
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EXECUTIVE SUMMARY

The Kristin Jacobs Coral Reef Ecosystem Conservation Area (Coral ECA) Water Quality Assessment (WQA) was designed in 2014 by a collaborating body of National Oceanic and Atmospheric Administration (NOAA) scientists, Florida Department of Environmental Protection's Coral Reef Conservation Program (CRCP) staff, and partners from the Southeast Florida Coral Reef Initiative (SEFCRI). The goal of the WQA was to provide data for managers to assess the status of the Coral ECA, an area which historically did not have a consistent water quality monitoring program.

The focus of this study extends from the St. Lucie Inlet in the north to offshore Biscayne Bay in the south, containing nine major inlets, namely, St. Lucie (STL), Jupiter (JUP), Lake Worth (ILW), Boynton (BOY), Boca Raton (BOC), Hillsboro (HIL), Port Everglades (PEV), Baker's Haulover (BAK), and Government Cut (GOC).

The overall goal of this assessment is to identify both the constituents and impacts of land-based sources of pollution on coral reef ecosystems and inform resource managers and decision-makers on the water quality status in the Southeast Florida coastal zone. Our objectives in that context are aimed to answer the following questions:

1. Does water quality differ among ICAs?

Yes, water quality is different among the various ICAs and is driven by geographical location, distance from shore, terrestrial runoff, freshwater input, etc. This is confounded by the composition of "Site Types" (Inlet, Outfall, & Reef) within each ICA. Some ICAs include Outfall sources (BAK, BOC, GOC, HIL, & PEV), some ICAs are dominated by large freshwater inlets (BOC, HIL, JUP, and especially STL). ILW sites are classified as Inlet and Reef but they are all low in nutrients with high optical clarity so look more like other Reef areas. Whereas, the STL sites have high nutrients, low salinity, and poor optical clarity and therefore look more like Inlet than Reef. The take home message is that we should let the data inform site classifications rather than comparing apples to oranges.

2. Does water quality differ among Site Types (Inlet, Outfall, and Reef)?

Yes, water quality is different among "Site Types", but these categories have been subjectively applied to sampling sites. Objective analyses (PCA, MDS, and Cluster analysis) showed, with a few exceptions, that the classifications were distinct enough to be statistically different. Inlet sites all had similar water quality except for the STL, which was significantly different than other Inlets. The STL Reef sites clustered with other Inlet sites. Conversely, the ILW Inlet water quality clustered with other Reef sites. For future analyses, FDEP might want to reclassify some Site Types to be more consistent.

3. Does water quality differ between surface and bottom waters?

Yes, water quality is typically significantly different between surface and bottom samples from the same site. Variables most different tend to be those land-derived variables such as nutrients and sediments. These differences are complicated by current patterns and density stratification. Freshwater inputs from Inlets tend to remain at the surface rather than mix with depth. These areas also tend to have higher surface nutrient inputs. Outfall water sources enter at the bottom of the water column and are fresher than seawater. This means outfall sources tend to be buoyant and mix sewage nutrients throughout the water column.

4. How Do Available Water Quality Data Compare to Relevant Published Benchmarks, Especially Those of SE Florida Waters?

Scientific Consensus Approach: The purpose of this Task is to provide a scientifically defensible methodology to ultimately assist FDEP in the development of biogeochemically relevant benchmarks for the ECA. We provide a compendium of those studies which strived to summarize these effects and draw a 'line in the water' by establishing water quality benchmarks/thresholds/criteria to further the continued growth, development, and survival of coral reefs.

Early work in the 60's and 70's was mostly observational, much like Hart (1974). More refined empirical and nutrient dosing field studies provided the foundation for most governmental standards and criteria e.g., ANZECC, ARMCANZ (2000), GBRMPA (2009), FDEP (2013), Hawai'i State Department of Health (2021). Smith's pioneering work in Kaneohe Bay (1977) fired the starting gun for more in situ and lab-based studies.

For laboratory-based, experimental studies, the question has always been, what is the best measure to assess 'impact'? Some researchers have used rate of coral growth, some used mortality, and others used everything else in between. Bradley et al. (2010) provided a relevant discussion in relating the Clean Water Act to biocriteria as well as water quality criteria for coral reefs.

A recent meta-analysis on lab-based, experimental nutrient effects to corals by Nalley et al. (2023) attempted to address this multiple response problem by "classifying effects of DIN (nitrate and ammonium) and DIP (phosphate)" into nine physiological "coral holobiont responses":

A. Photosynthetic responses of the coral endosymbiont
   1. Zooxanthellae density
   2. Chl-a concentration
   3. Photosynthetic rate
   4. Photosynthetic efficiency (max. quantum yield)

B. Coral growth and calcification

1. Growth rate
2. Calcification rate

C. Mortality

1. Adult tissue and colony survival
2. Larval survival and settlement
3. Fertilization success

We believe that the value of the many empirical studies and field dosing experiments, being more inclusive of the coral community, should not be discounted and have therefore given more weight to this body of work for benchmark development. Our ‘suggested’ Scientific Consensus of the published benchmarks is described in Task 2.1b and summarized in the following Table *i*.

EPA 75th Percentile Approach: EPA recommends a reference site approach for setting benchmarks (US-EPA 2001) where sites are selected based on minimal human influence. If values from other sites fall within an acceptable range of reference sites (typically 75th percentile) they are considered to meet the designated use. In some areas minimally disturbed reference conditions do not exist and may not be achievable. In these situations, “least disturbed sites” may be used (25th percentile) if they demonstrate that the existing biological community structure and function is representative of a sustainable, natural system. Results of 75th Percentile analysis are shown in Table *i*.

CUSUM Approach:

Given the large proportion of non-detects in the ECA water quality database, we could not derive benchmarks using the cumulative sum method (Briceño et al. 2010; Regier et al. 2019). Instead, we used data gathered during the 2009-2012 period for the same ECA study area, from the Southeast Florida Coral Reef Initiative (SEFCRI) project (Boyer 2012). This method entails plotting CUSUM-transformed CHL*a* data against potential drivers to extract meaning in the context of driver-response relationships.

Benchmark Approach Comparison: The three separate benchmark approaches are compared in Table *i*. The 75th percentiles for total ECA compare relatively well with the Scientific Consensus benchmarks except that DIN values were higher and Secchi depth was lower in the ECA than proposed by Scientific Consensus. CUSUM benchmarks compare well with Scientific Consensus and 75th Percentile approaches but were slightly lower overall.

Variable	Consensus	75th percentile	Cluster 1	Cluster 2	Cluster 3	Cluster 4
$NH4^+$ (ppb)	**5**	**13**	7	2	4	4
$NO3^-$ + $NO2^-$ (ppb)	**5**	**8**	4	2	4	7
DIN (ppb)	**10**	**21**	11	8	9	8
$PO4^-$ (ppb)	**3**	**2**	2	1	1	1
TN (ppb)	**150**	**69**	133	96	97	118
TP (ppb)	**10**	**10**	6	5	6	5
CHLa (µg)	**0.3-0.5**	**0.6**	0.4	0.3	0.5	0.4
Turbidity (NTU)	**0.5**	**0.6**	0.4	0.1	0.1	0.5
TSS (ppm)	**10**		a	a	a	a
Secchi (m)	**10**	**8.5**	a	a	a	a
Kd (m^{-1})	**0.14**		0.12	0.06	0.09	0.13

Table i. *Benchmark Approach Comparison of Scientific Consensus, 75th Percentile, and CUSUM from 4 distinct site clusters. Demarcation "a" means insufficient or no data.*

5. Recommendations

We have three general recommendations concerning this project moving forward. The first reiterates a recommendation from our previous report (Briceño et al. 2022) that FDEP should work to reduce the number of non-detects in future laboratory analyses. This means either upgrading the existing laboratory sensitivity for low level nutrient analyses or by using a different contract laboratory with higher analytic sensitivity.

The second recommendation concerns treatment of non-detect data. Censored maximum likelihood estimation is an efficient method to estimate the distributions, taking account of the observations below the MDL. If more readings can be obtained over the MDL then different estimation methods will become more similar, and ideally the analysis should not be very sensitive to the choice of estimation method.

The third recommendation concerns derivation of water quality benchmarks. Each approach, the Scientific Consensus, 75th Percentile, and CUSUM, are valid methods in their own right. Surprisingly, the results of all three approaches for the ECA water quality were similar for NO3+NO2, PO4, CHLa, turbidity, and Secchi depth. The Scientific Consensus result was lower for NH4 but higher than the other two approaches for TN and TSS.

We believe that the choice of which benchmark approach to use for the ECA should be debated by the local coral reef scientific and regulatory community. There are advantages and disadvantages for each method.

Advantages of the Scientific Consensus are that there is considerable weight of evidence generated from the many peer-reviewed studies and that these results all fall within a relatively narrow range. The disadvantages include inherent variability in laboratory analyses, fluctuations in geographical ambient nutrient levels, global differences in coral community structure, etc.

An advantage of the 75th Percentile approach is that it uses data generated from the local area of interest. It may also be used to mine historical data. Conversely, the main disadvantage of the 75th Percentile approach is that it relies on data collected from the local area of interest. If the area of interest is already impacted, the benchmarks will be overestimated. However, future benchmarking could be refined by more selective use of least-impacted ICAs. The PC/MDS/Cluster analyses showed that data from most Inlets should be excluded from the computation because they are very different than Reef sites. Conversely, the ILW might be included in REEF as its water quality was comparable with other Reef sites. Outfall sites are problematic because they typically occur farther from shore and in deeper waters than Reefs (2.1-17.1 m vs 16.8-54.9 m). In addition, there is no data collected at bottom Outfall sites where impacts may be expected.

The CUSUM approach also relies on local data but has the advantage in that it quantifies a driver-response threshold for increase in CHLa production (phytoplankton biomass). The disadvantage is that, currently, there are no other driver-response effects in place for coral reef impacts which occur at the same time scale of water quality sampling events. Lags between driver-response reduce the ability to resolve thresholds.

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BACKGROUND

The counties of Southeast Florida (Miami Dade, Broward, Palm Beach, and Martin) are highly urbanized and inhabited by 6.3 million people. Most development occurs directly along the coast, and Florida's Coral Reef lies to the east, just 1.5 km from the urbanized shoreline. Therefore, southeast Florida's coral reefs are directly impacted by anthropogenic stressors, especially terrestrial runoff, and from failing wastewater disposal systems, which degrade coastal water quality.

The Kristin Jacobs Coral Reef Ecosystem Conservation Area (Coral ECA) Water Quality Assessment (WQA) was designed in 2014 by a collaborating body of National Oceanic and Atmospheric Administration (NOAA) scientists, Florida Department of Environmental Protection's Coral Reef Conservation Program (CRCP) staff, and partners from the Southeast Florida Coral Reef Initiative (SEFCRI). The goal of the WQA was to provide data for managers to assess the status of the Coral ECA, an area which historically did not have a consistent water quality monitoring program.

The overall goal of this assessment is to identify both the constituents and impacts of land-based sources of pollution on coral reef ecosystems and inform resource managers and decision-makers on the water quality status in the Southeast Florida coastal zone. Our objectives in that context are aimed to answer the following questions:

1) Are there differences in the data between the individual ICA's?
2) Are there differences between site types – inlet, outfall and reef samples?
3) Is there a significant difference in analyte concentrations between bottom vs surface samples?
4) How do the available concentration data compare to any relevant published benchmarks, especially to those of SE Florida waters?

The focus of this study extends from the St. Lucie Inlet in the north to offshore Biscayne Bay in the south, containing nine major inlets, namely, St. Lucie (STL), Jupiter (JUP), Lake Worth (ILW), Boynton (BOY), Boca Raton (BOC), Hillsboro (HIL), Port Everglades (PEV), Baker's Haulover (BAK), and Government Cut (GOC) (Fig 1).

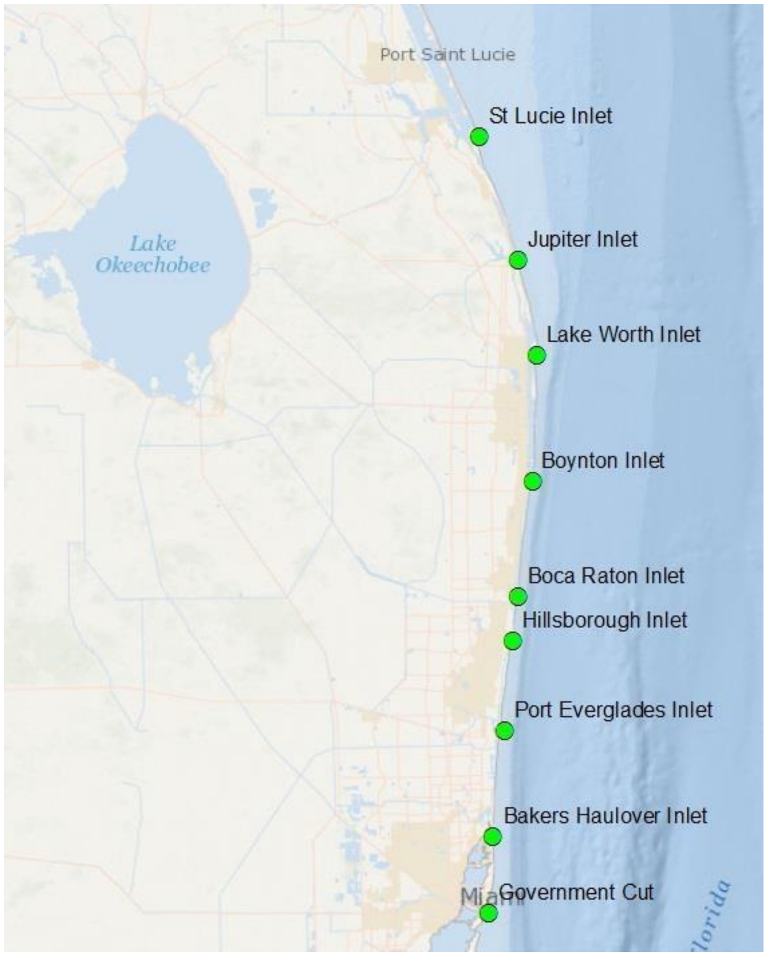


***Figure 1**. Map of study area, showing the location of Inlet Contributing Areas (ICAs). From Whitall et al. 2019*

TASK 1: Statistical Analysis Among ICAs, Site Types, and Depths

Statistical analyses were carried out to investigate differences between compositional and physical-chemical measures among:

1. Individual ICAs,
2. Site-types (inlet, reef, outfall),
3. Surface and bottom characteristics.

In this initial phase, appropriate statistical methods were used to address uncertainty and consider the variety of detection limits that are present in the dataset. In particular, statistical models and methodology for dealing with censored data for handling the non-detected values were employed in this task. We present exploratory data analysis using plots and numerical statistics; maximum likelihood estimation using Weibull models. Albeit log-normal or other appropriate models, and non-parametric methods such as permutation tests may be used, likelihood-based methods are the most efficient estimation and testing procedures (Helsel 2005; Hewett, P. and H. Ganser. 2007; Jain et al. 2008). Test results are presented below to give concise numerical and visual findings.

Does Water Quality Differ Among ICAs?

Originally, the ECA water quality database contained results from analysis of Broward County Environmental Monitoring Laboratory and Texas A&M Geochemical and Environmental Reserach Group (GERG) laboratories. Upon recommendation of FDEP, we consider the data from the Broward laboratory without including the GERG laboratory values in this report. In Table 1 we present the number of observations and in Table 2 the percentage of detected values which are above the Method Detection Limit (MDL).

The variables collected are: NH_4 (ammonium), NO_3 (nitrate), NO_2 (nitrite), NO_X (nitrate + nitrite), TKN (total Kjeldahl nitrogen), PO_4 (orthophosphate), TP (total phosphorus), CHL*a* (chlorophyll *a*), TSS (total suspended solids), SAL (salinity), SiO_4 (silicate), TOC (total organic carbon), Secchi depth and TURB (turbidity). After each measure, S indicates a measure taken at the surface waters, and B is a measure taken at the bottom waters. From Table 1 we see that there are no observations for bottom water measures at Outfall sites. Also, there are very small sample sizes for TOC.

no of observations

	In GOC	In BAK	In PEV	In HIL	In BOC	In BOY	In ILW	In JUP	In STL	Reef GOC	Reef BAK	Reef PEV	Reef HIL	Reef BOC	Reef BOY	Reef ILW	Reef JUP	Reef STL	Out GOC	Out BAK	Out PEV	Out HIL	Out BOC
NH4.S	140	204	204	208	208	204	204	204	140	245	305	306	312	312	408	306	306	280	140	204	204	208	208
NH4.B	140	204	156	208	208	204	204	204	140	245	306	234	312	312	408	306	282	280	0	0	0	0	0
CHLA.S	92	92	92	94	94	92	94	94	94	137	121	122	124	124	152	126	126	158	74	74	74	75	75
CHLA.B	60	60	60	60	60	60	64	64	64	109	94	94	94	91	124	100	100	132	0	0	0	0	0
Secchi	140	203	203	206	205	204	202	199	139	245	303	304	309	308	408	302	306	280	98	151	108	154	154
NO3.S	140	203	204	208	208	204	204	204	140	245	306	306	312	311	408	306	306	280	140	204	204	208	208
NO3.B	140	204	156	207	208	204	204	204	140	245	306	234	312	312	408	306	282	280	0	0	0	0	0
NOX.S	140	204	204	208	208	204	204	204	140	245	306	306	312	311	408	306	306	280	140	204	204	208	208
NOX.B	140	204	156	208	208	156	204	204	140	245	306	234	312	312	389	306	282	280	0	0	0	0	0
NO2.S	140	204	204	208	208	204	204	204	140	245	306	306	312	312	408	306	306	280	140	204	204	208	208
NO2.B	140	204	156	208	208	204	204	204	92	245	306	234	311	312	408	306	282	280	0	0	0	0	0
TKN.S	140	204	204	208	208	204	204	204	140	245	306	306	312	312	408	306	306	280	140	204	204	206	208
TKN.B	140	204	156	208	208	204	204	204	140	245	306	234	312	312	408	306	282	280	0	0	0	0	0
PO4.S	140	204	204	208	208	204	204	204	140	245	306	306	312	312	408	306	306	280	140	204	156	208	208
PO4.B	140	204	156	208	208	204	204	204	140	245	306	234	312	312	408	306	282	280	0	0	0	0	0
TP.S	140	204	204	208	208	204	204	204	140	245	306	306	312	312	408	306	306	280	140	204	156	207	208
TP.B	140	204	156	208	208	204	204	204	140	245	306	234	312	312	408	306	282	280	0	0	0	0	0
TSS.S	140	204	204	208	208	204	204	204	140	245	306	305	312	312	408	306	306	280	140	204	156	208	208
TSS.B	140	204	156	208	208	204	204	204	140	245	306	234	312	312	408	306	282	280	0	0	0	0	0
SAL.S	140	204	204	207	208	202	204	203	134	241	305	301	310	311	407	300	305	278	140	203	154	206	207
SAL.B	140	204	156	208	208	204	204	204	140	242	304	229	311	308	406	306	281	279	0	0	0	0	0
SiO4.S	140	204	196	208	208	204	204	204	140	245	306	304	312	312	408	306	306	280	140	204	156	207	208
SiO4.B	140	204	150	208	208	204	204	204	140	245	306	231	311	312	408	306	282	280	0	0	0	0	0
TOC.S	8	8	8	8	8	8	8	8	8	14	12	12	12	12	16	12	12	16	8	8	8	8	20
TOC.B	8	8	8	8	8	8	8	8	8	14	12	12	12	12	16	12	12	16	0	0	0	0	0
TURB.S	140	204	204	208	208	204	204	204	140	245	306	306	312	312	408	306	306	280	140	204	156	208	196
TURB.B	140	204	156	208	208	204	204	204	140	245	306	234	312	312	408	306	281	280	0	0	0	0	0

Table 1: *Number of observations for the variables at each ICA/Type. The colors represent Blue for higher values and Red for lower values. Locations are ordered from south to north.*

Table 2 shows there are many variables with very few/zero detected values above the MDL. This causes methodological problems for the estimation of any quantities from the distribution of variables. However, we shall proceed with a censored maximum likelihood method for estimating the upper quartiles of the measures.

% detected

	In GOC	In BAK	In PEV	In HIL	In BOC	In BOY	In ILW	In JUP	In STL	Reef GOC	Reef BAK	Reef PEV	Reef HIL	Reef BOC	Reef BOY	Reef ILW	Reef JUP	Reef STL	Out GOC	Out BAK	Out PEV	Out HIL	Out BOC
NH4.S	72.9	39.2	45.6	45.2	53.4	40.7	39.7	39.7	62.1	56.3	35.7	34.3	40.7	41.7	34.8	35.6	31	50.4	77.1	57.8	53.4	58.7	55.3
NH4.B	67.1	34.8	32.7	32.2	38	32.8	35.3	37.7	54.3	46.5	33.7	30.8	28.2	30.1	31.6	33	35.5	48.6					
CHLA.S	100	100	100	98.9	97.9	100	98.9	100	100	98.5	98.3	100	99.2	98.4	96.1	98.4	98.4	99.4	93.2	93.2	98.6	89.3	97.3
CHLA.B	100	100	98.3	100	100	100	100	100	100	95.4	100	98.9	100	100	97.6	100	100	100					
Secchi	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
NO3.S	41.4	26.1	47.1	28.4	35.6	14.2	13.7	11.3	25	15.5	21.2	18.3	19.9	15.1	7.8	10.5	9.5	17.9	8.6	22.5	27.9	26.4	20.7
NO3.B	31.4	23	10.9	20.3	20.7	7.4	9.8	11.8	27.1	15.9	20.6	13.7	17.6	10.3	12.7	13.1	16.7	21.1					
NOX.S	57.1	44.1	61.8	41.8	45.7	27.5	20.1	28.9	37.1	31	36.6	29.7	36.2	30.5	18.1	20.6	17.3	24.6	47.1	50	40.7	49.5	37.5
NOX.B	55	37.7	28.2	38	34.6	16	19.6	28.9	34.3	31.4	45.1	26.9	33.3	24.4	30.3	21.2	27	33.6					
NO2.S	7.1	9.3	16.2	12.5	15.9	11.8	8.8	9.8	14.3	7.3	7.5	8.5	9.3	9	9.1	8.2	7.2	7.9	40	30.9	28.9	35.1	25
NO2.B	4.3	7.4	10.3	10.1	12.5	7.8	8.3	8.8	13	4.1	7.5	10.7	7.4	6.1	9.8	8.2	8.2	4.6					
TKN.S	61.4	30.9	35.8	35.1	42.8	36.3	16.7	40.7	68.6	26.9	15.7	11.8	22.4	23.7	8.6	13.1	12.1	48.2	60	31.9	25	35.4	28.8
TKN.B	48.6	25.5	10.9	20.7	24.5	23.5	10.3	34.8	60.7	22.4	12.7	10.3	12.2	14.7	7.8	13.7	11	40.4					
PO4.S	0.7	0	5.9	19.2	32.2	12.7	6.4	12.3	56.4	1.2	0.3	1	2.9	8	2.9	3.6	5.9	33.2	42.9	24	28.2	18.8	26.9
PO4.B	0	0	0	4.3	14.9	4.9	3.9	8.3	45.7	0.8	0.3	0	1.9	3.2	0.2	4.2	4.6	22.5					
TP.S	2.1	8.8	5.9	4.3	13.5	9.3	6.9	8.8	42.9	0	8.2	7.8	7.4	7.4	7.4	5.2	7.8	21.8	30	12.7	22.4	10.1	18.3
TP.B	1.4	9.3	5.8	5.3	9.6	6.9	5.4	8.8	32.1	1.2	8.8	8.1	4.8	4.2	7.4	4.6	8.2	18.9					
TSS.S	27.9	27.9	25.5	27.9	26.4	32.8	27	45.1	62.1	17.6	19	24.3	25.3	23.7	20.1	29.4	26.8	43.2	20.7	16.7	27.6	28.4	17.3
TSS.B	26.4	24	23.1	23.1	22.1	22.5	30.9	38.2	53.6	20	16.7	22.2	23.7	20.8	22.1	29.1	24.1	47.1					
SAL.S	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
SAL.B	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100					
SiO4.S	92.1	88.7	78.1	80.3	78.8	65.7	52	72.5	92.9	60.8	65.7	63.5	66	65.4	48	35.3	44.1	79.3	67.1	59.3	59.6	61.8	66.3
SiO4.B	90.7	83.8	57.3	65.4	60.1	54.4	43.6	60.8	89.3	53.5	53.3	64.1	47.9	52.2	47.5	35.6	45	78.9					
TOC.S	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
TOC.B	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100					
TURB.S	100	100	100	100	100	100	100	100	100	100	100	100	100	100	98.5	100	99.7	100	100	99.5	99.4	97.6	98.5
TURB.B	100	100	100	100	100	98.5	99.5	100	100	100	100	100	100	99.7	99.5	100	100	100					

Table 2: *The percentage of observations above the Method Detection Limit (MDL). Blue are high percentages and red are low. The gray values have no observations (value 0 in Table 1).*

Upper Quartile Estimation. Weibull censored MLE upper quartiles

We compared the estimated upper quartile (75th percentile) for the variables at different ICA/ type sites (Table 3). The upper quartiles for all variables except SAL, and Secchi were estimated using Maximum Likelihood Estimation (MLE) for a two parameter Weibull distribution with left censoring for values below the MDL. Results from our previous work in this project indicated that for highly censored datasets, the Weibull MLE was the best overall estimator (Briceño et al. 2022).

For SAL and Secchi with no censored values, we use the empirical upper quartiles rather than the Weibull distribution. The logarithms of the estimated upper quartiles are used in the following statistical analysis, standardized over the surface (S) and bottom (B) values for each measure.

As already noted for some of the sites there were very few and sometimes zero values above the MDL. Also, the method is dependent on the Weibull distribution being an appropriate probability distribution for the measurements. From earlier analysis, probability plots for the Weibull were often appropriate when available, and the censored MLE method has previously been suggested as a good choice (Briceño et al. 2022). Nonetheless estimated quartiles are uncertain, and so this must be borne in mind when interpreting results. The statistical analysis would be improved by having lower MDL with a higher percentage detection rates. Also, samples taken at the bottom of Outfall sites would improve future analysis.

Summary: Yes, water quality is different among the various ICAs and is driven by geographical location, distance from shore, terrestrial runoff, freshwater input, etc. This is confounded by the composition of "Site Types" (Inlet, Outfall, & Reef) within each ICA. Some ICAs include Outfall sources (BAK, BOC, GOC, HIL, & PEV), some ICAs are dominated by large freshwater inlets (BOC, HIL, JUP, and especially STL). ILW sites are classified as Inlet and Reef but they are all low in nutrients with high optical clarity so look more like other Reef areas. Whereas, the STL sites have high nutrients, low salinity, and poor optical clarity and therefore look more like Inlet than Reef. The take home message is that we should let the data inform site classifications rather than comparing apples to oranges.

Does Water Quality Differ Among Site Types (Inlet, Reef, & Outfall)?

Exploratory analysis is carried out to compare the ICA Site Types (Inlet, Outfall and Reef) using the estimated upper quartiles for the variables. For the subsequent analysis we standardize each log-variable over the available sites (subtract mean and divide by standard deviation of the pooled surface/bottom values for each variable) to eliminate the influence of magnitude disparities among variables. The estimated upper quartiles are given in Table 3, with coloring according to the standardized log values (ranging from -3.3 to 4.2).

	In GOC	In BAK	In PEV	In HIL	In BOC	In BOY	In ILW	In JUP	In STL	Reef GOC	Reef BAK	Reef PEV	Reef HIL	Reef BOC	Reef BOY	Reef ILW	Reef JUP	Reef STL	Out GOC	Out BAK	Out PEV	Out HIL	Out BOC
NH4.S	16.27	11.67	14.64	16.56	22.32	14.59	12.9	12.52	15.34	14.62	10.95	10.06	12.04	13.61	11.51	10.99	9.51	11.57	212.39	39.34	50.16	70.64	38.83
NH4.B	15.66	10.56	8.17	9.62	13.73	10.47	10.32	11.96	13.34	11.08	9.9	7.41	8.18	9.11	10	10.1	10.76	11.01					
CHLA.S	0.76	1.24	1.58	1.67	1.49	1.93	0.9	1.91	2.62	0.67	0.74	0.76	1.22	0.97	0.76	0.56	0.61	1.43	0.55	0.63	0.45	0.6	0.61
CHLA.B	0.79	1.16	0.63	1.2	0.83	1.02	0.56	1.31	1.72	0.62	0.73	0.56	0.87	0.6	0.46	0.48	0.62	1.13					
Secchi	6	5	7	4.82	4.3	6	7.9	4	3	7.9	7.6	8.5	6.71	4.6	15	4	12.14	5	13	13	15	13.92	14.37
NO3.S	11.48	8.54	16.74	10.04	12.89	3.77	3.41	4.42	7.48	4.59	7.18	6.37	6.22	4.59	3.69	3.88	3.78	5.46	2.01	7.07	10.63	8.67	6.54
NO3.B	8.86	7.68	4.07	6.9	6.22	3.18	3.95	4.45	8.26	5.91	6.73	5	6.16	5.1	4.02	4.95	5.33	6.54					
NOX.S	12.81	10.41	18.81	12.05	14.14	6.02	4.01	6.58	9.62	6.39	8.42	7	8.29	7.06	4.33	4.7	3.9	5.46	12.33	15.39	16.09	15.81	10.94
NOX.B	10.22	8.81	5.99	8.63	8.18	3.67	4.41	6.49	8.88	6.49	9.88	5.82	7.16	5.72	6.43	4.87	6.41	7.34					
NO2.S	0.85	0.51	1.58	1.05	1.45	0.62	0.34	0.52	1.05	0.71	0.26	0.4	0.57	0.41	0.33	0.27	0.21	0.7	5.95	4.26	4.17	5.58	3
NO2.B	0.74	0.25	0.46	0.76	0.91	0.16	0.3	0.38	0.88	0.56	0.26	0.51	0.32	0.13	0.37	0.27	0.25	0.19					
TKN.S	0.08	0.06	0.07	0.08	0.09	0.08	0.03	0.09	0.13	0.04	0.03	0.03	0.04	0.05	0.01	0.03	0.02	0.07	0.27	0.07	0.02	0.1	0.06
TKN.B	0.07	0.05	0.02	0.04	0.05	0.05	0.02	0.07	0.11	0.04	0.03	0.02	0.03	0.03	0.02	0.03	0.02	0.06					
PO4.S	1.15		0.88	3.49	6.14	1.56	0.51	1.78	13.45	0.04	0	0	0.68	0.63	0.5	0.68	0.49	6.03	12.87	4.33	6.38	2.82	5.24
PO4.B				1.13	2.13	1.26	0.2	0.85	9.43	0.27	0		0.42	0.3	0.13	0.27	1.63	3.8					
TP.S	0.4	1.02	0.47	1.36	7.57	1.54	6.65	3.33	22.85		0.75	1.31	4.24	2.75	0.52	4.91	0.91	13.85	18.91	3.63	15.2	6.41	10.97
TP.B	0.12	1.16	0.28	4.26	4.23	0.36	1.41	2.12	18.25	0.19	1.06	1.27	0.67	3.27	0.6	3.78	1.06	11.12					
TSS.S	3.89	3.55	3.22	3.52	3.41	4.92	3.86	8.15	7.33	2.26	1.66	3.02	3.1	2.83	1.77	4.38	3.47	5.44	2.91	1.35	4.1	3.9	1.51
TSS.B	3.64	2.59	2.82	2.58	2.51	2.13	5.19	6.44	6.78	2.8	1.34	2.52	2.59	2.24	2.14	4.33	2.84	6.93					
SAL.S	35	36	35	36	36	35	36	35	35	36	36	36	36	36	36	36	36	36	36	36	36	36	36
SAL.B	36	36	36	36	36	36	36	36	36	36	36	36	36	36	36	36	36	36					
SiO4.S	0.08	0.11	0.17	0.22	0.19	0.09	0.04	0.13	0.28	0.03	0.04	0.05	0.08	0.06	0.02	0.01	0.03	0.13	0.07	0.03	0.04	0.05	0.07
SiO4.B	0.06	0.08	0.03	0.06	0.06	0.04	0.02	0.07	0.2	0.02	0.02	0.03	0.02	0.03	0.02	0.01	0.02	0.09					
TOC.S	1.6	1.55	1.83	2.25	2.48	1.19	1.59	2.56	4.19	1.24	1.29	1.35	1.55	1.43	1.13	1.28	1.09	2.86	1.22	1.19	1.41	1.17	0.87
TOC.B	1.25	1.46	1.1	1.81	1.93	1.12	1.38	2.08	3.07	1.04	1.08	1.14	1.22	1.1	1.08	1.26	1.12	1.61					
TURB.S	1.17	1.15	0.92	0.68	0.82	1.03	0.92	1.96	3.3	0.52	0.59	0.66	0.56	0.58	0.33	0.74	0.6	2.13	0.44	0.38	0.34	0.34	0.3
TURB.B	1.16	1.21	0.46	0.56	0.64	0.73	1	1.84	3.2	0.51	0.57	0.59	0.45	0.52	0.34	0.84	0.8	2.87					

key: 4, 2, 0, -2

Table 3. *Estimated upper quartiles (75th percentiles) using Weibull censored MLE for most variables and empirical upper quartiles for SAL, Secchi. The coloring for each variable (in each pair of rows for S and B where available) is from the standardized log variables where the mean of the log values is 0 and the variance is 1. The colors represent Blue for lower values and Red for higher values. The gray values are where quantile estimates are not available due to either no observations or low sample size.*

Some observations from Table 3.

- The Reef sites generally have lower values of all upper quartiles, except SAL. The Reef at STL does not fit this pattern, having values more similar to an Inlet site.
- Outfall sites generally have some higher nutrient analyte concentrations (NH4, NO2, PO4, TP), higher Secchi and lower CHLA, SiO4, TOC, TURB than Inlet sites.
- Inlets sites BOY, ILW, JUP have generally lower NO3, NOX, NO2 values than the other Inlet sites.
- SAL.S at Inlets contains some lower values than Reef and Outfall.
- STL Inlet has very high values for almost everything except Secchi and SAL.

<u>Principal Components Analysis</u>

To explore the differences between ICA Site Types and the relationship between the variables we used principal components analysis (PCA). The standardized logarithm of estimated upper quartiles is treated as data, with the values in gray in Table 3 as missing. In fact, we imputed these missing values using variable means, because to compute the PCA for Outfall sites one must have something to multiply by the Variable.B coeffients in order to compute the PC score. If you impute with the mean of the variable then the coefficient is multiplied by zero. It is the same as ignoring the grey values, as we should.

The principal component loadings are given in Table 4 where we highlight factor loadings above 0.20 in order to provide some interpretation of "relatedness" among variables. For example, PC1 had the highest factor scores for CHLA, TKN, PO4, SiO4, TOC, and Turb. In contrast, PC2 showed that surface CHLA was inversely related to NH4, Secchi depth, NOX, NO2, and SAL.

	PC1	PC2	PC3		PC1	PC2	PC3
NH4.S	0.13	-0.42	-0.08	PO4.B	0.18	-0.04	-0.05
NH4.B	0.07	-0.14	-0.04	TP.S	0.16	-0.14	-0.32
CHLA.S	0.21	0.31	0.13	TP.B	0.17	-0.08	-0.27
CHLA.B	0.23	-0.05	-0.01	TSS.S	0.2	0.23	-0.15
Secchi	-0.15	-0.31	-0.02	TSS.B	0.2	0.01	-0.29
NO3.S	0.14	-0.03	0.56	SAL.S	-0.2	-0.25	-0.23
NO3.B	0.09	-0.11	0.05	SAL.B	0	0	0
NOX.S	0.19	-0.27	0.41	SiO4.S	0.27	0.11	0.21
NOX.B	0.09	-0.15	0.11	SiO4.B	0.26	-0.08	-0.02
NO2.S	0.19	-0.36	0.08	TOC.S	0.27	0.23	0.01
NO2.B	0.1	-0.17	0.09	TOC.B	0.24	-0.05	-0.1
TKN.S	0.27	-0.08	0.02	TURB.S	0.2	0.32	-0.05
TKN.B	0.23	-0.08	-0.05	TURB.B	0.23	0.04	-0.23
PO4.S	0.23	-0.11	-0.12				
				%variability	36.9	25	12.7

Table 4. *The coefficients of the first three PCs, and percentage of variability explained by each component.*

Interpretation:

- PC1 shows a contrast between (+) Analytes/Water Quality Indicators (CHLA, TSS, SiO4, TOC, TURB, NH4, NO3, NOX, NO2, TKN, PO4, TP) & (-) SAL.S, Secchi, suggesting less polluted marine waters as compared to land sources.
- PC2 shows a contrast between (+) Water Quality Indicators CHLA.S, TSS.S, TOC.S, TURB.S and (-) nutrient levels (NH4, NO3, NOX, NO2, TKN, PO4, TP) and SAL.S/Secchi
- PC3 has particularly high weightings for (+) NO3.S, NOX.S, SiO4.S versus (-) TP, TSS, SAL.S, TURB.B.

Pairwise plots of the PC scores show the differences among the ICA sites and Types (Fig. 2,3, and 4). We see that the Outfall Sites are very similar (close together), and different from the rest (isolated cluster). The Reef sites are also similar to each other (close together) except Reef STL. The Inlet sites are more varied, with inlet ILW close to the Reefs and Inlet STL separate from others.

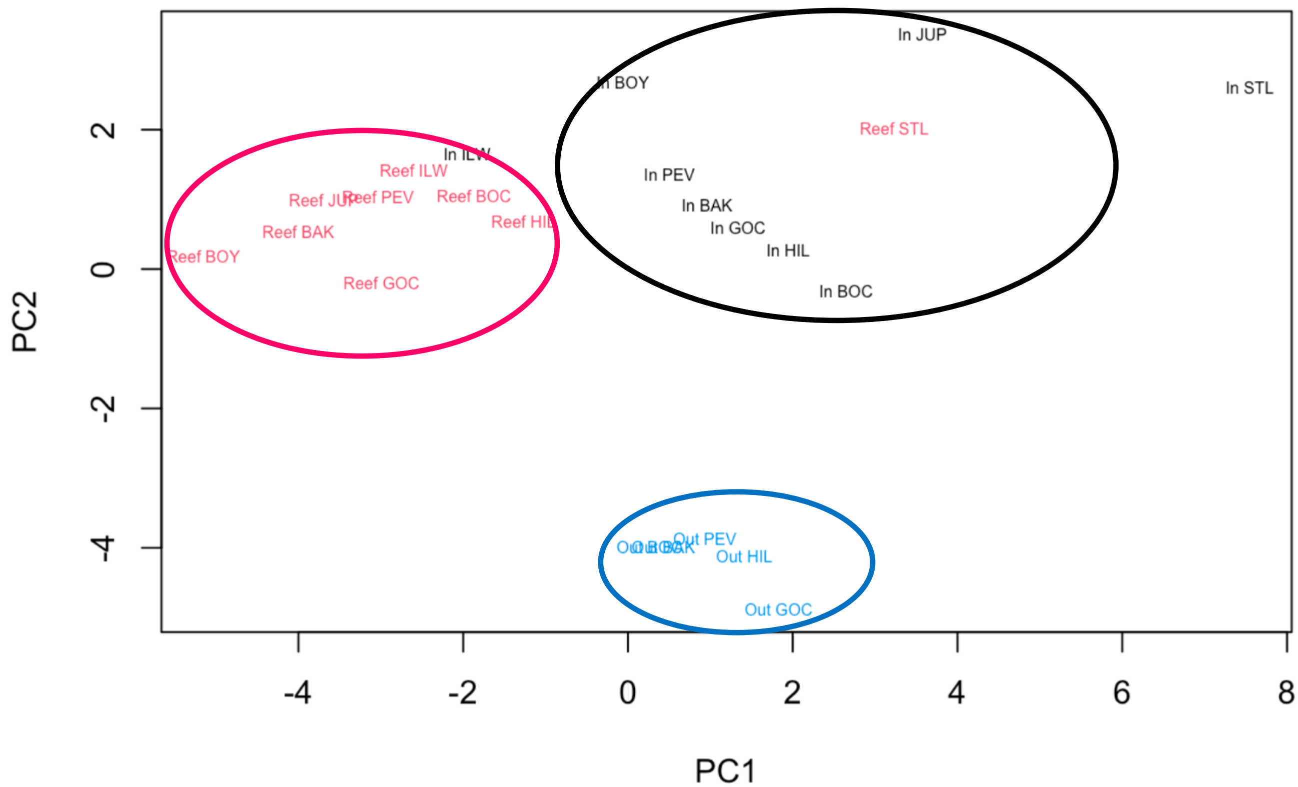


Figure 2. *A plot of PC score 2 versus PC score 1. The Inlet ICAs are black, the Reef ICAs in red, and the Outfall sites are blue.*

PC1 separates most Reef sites from Inlet and Outfall, except Reef STL and Inlet ILW. Relatively high values for SAL.S and Secchi with low values for other variables result in a low PC1 score for Reef sites (except STL). Note the very high values at Inlet STL and Reef STL for most variables (Table 3) leads to a very high PC1 score at these sites. The negative PC1 scores reflect better water quality and lower nutrient levels in the Reef sites (except STL). The positive PC1 scores reflect the worse water quality and higher nutrient levels seen in several Inlet sites.

PC2 separates the Outfall sites from the remainder (Fig. 3). We see that Outfall sites have very low PC2 and hence we expect lower CHLA.S, TSS.S, TOC.S, TURB.S, and higher nutrient analyte concentrations and SAL.S, Secchi values. Outfalls generally have high water clarity but also high nutrient levels (Table 3).

Note that PC3 primarily separates out Inlets PEV, HIL, BOC, BAK, GOC, Reef BAK as most positive scores and these all have relatively high NO3.S, NOX.S values (Fig. 3).

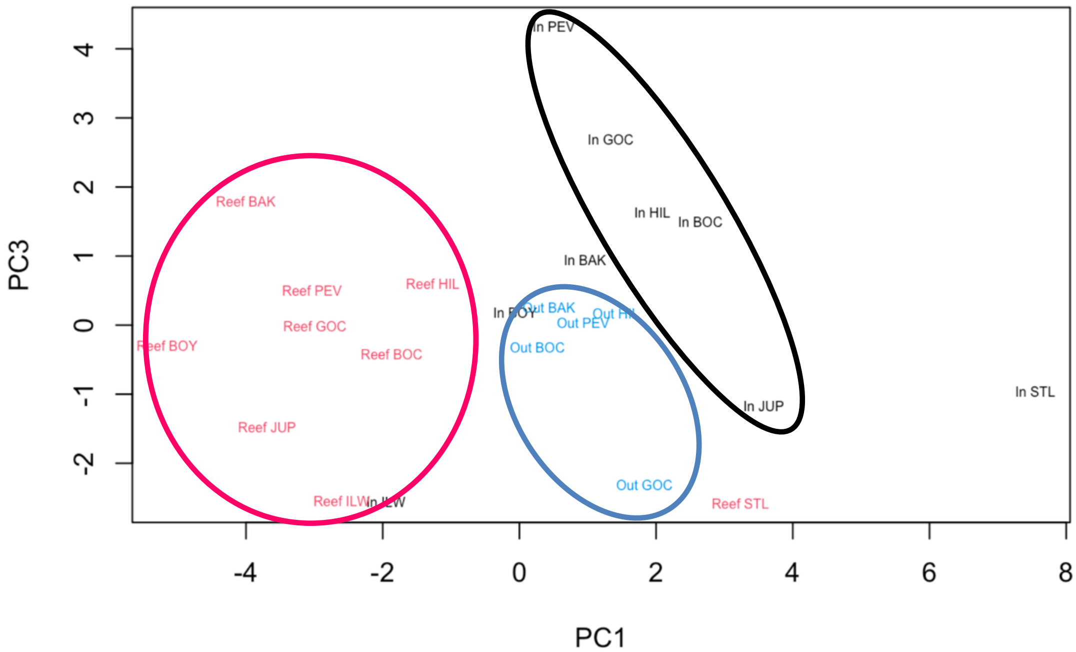


Figure 3. *A plot of PC score 3 versus PC score 1. The Inlet ICAs are black, the Reef ICAs in red, and the Outfall sites are blue.*

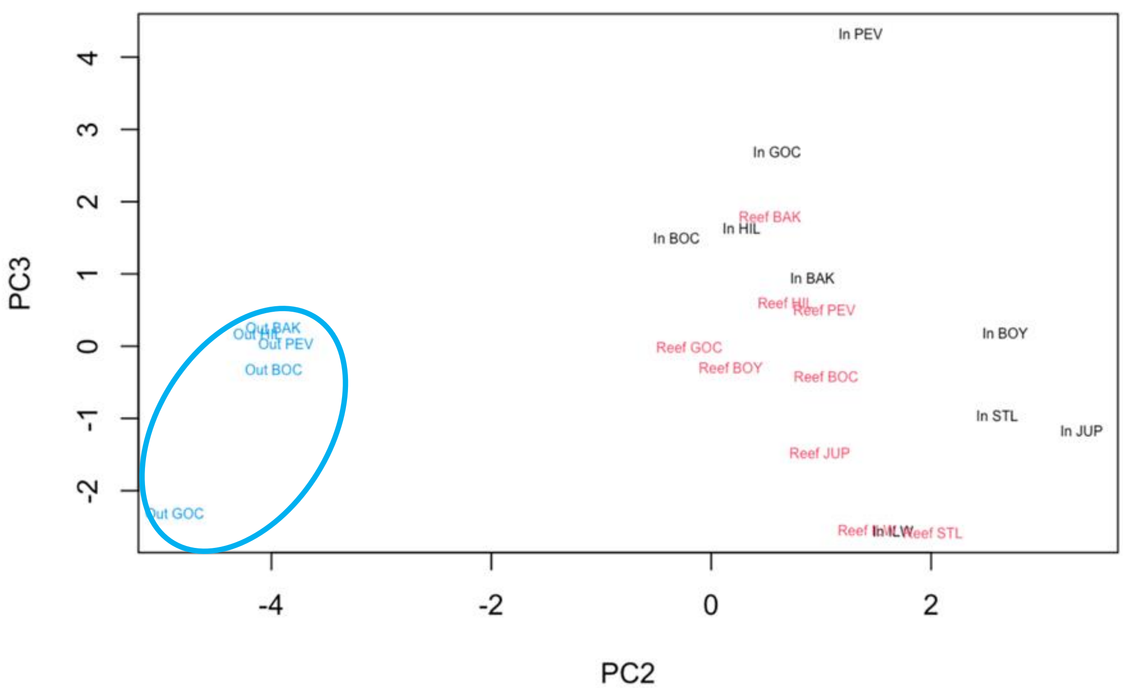


Figure 4. *A plot of PC score 3 versus PC score 2. The Inlet ICAs are black, the Reef ICAs in red, and the Outfall sites are blue.*

The percentage of variability captured by all PCS is shown in Figure 5. The first three PC scores account for 74.6% of the variability. Further analysis using additional PCs was not advised.

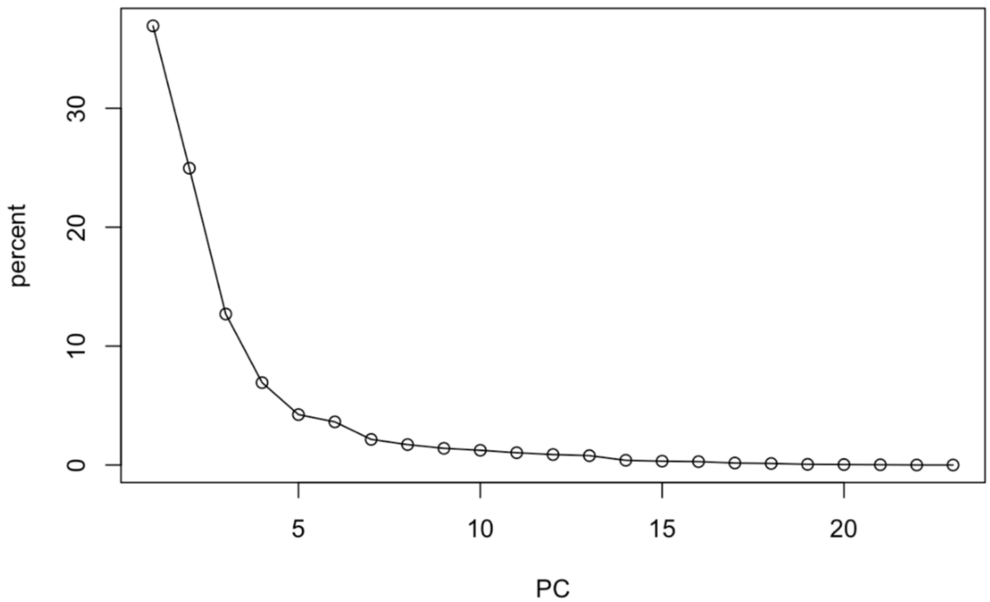


Figure 5: *The percentage of variability explained by each PC.*

Bi-plot

In Figure 6 we display a biplot which gives a visual display of the PC scores and loadings for PC1 and PC2. The red arrows in the biplot give information about the sign and weights of coefficients of the variables for each PC. A variable with vector pointing right horizontally has a very strong positive component in PC1, it would be negative if pointing left. If pointing up, a variable has a positive PC2 coefficient, if pointing down a strong negative PC2 coefficient. Other directions are weights of these coefficients, e.g., pointing up and right has positive PC1 and positive PC2 coefficients.

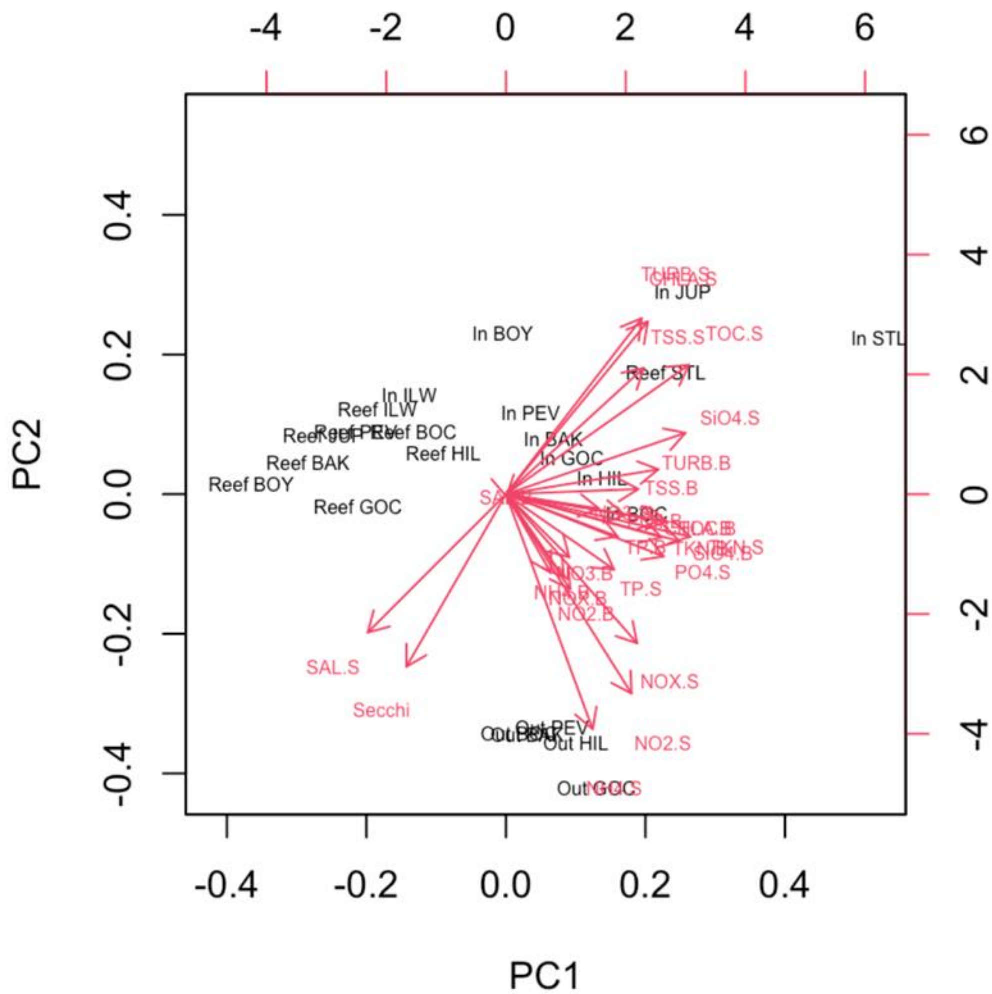


Figure 6. *Bi-plot for the PCA of the standardized log estimated upper quantiles.*

The biplot shows the PC scores again but also red arrows in the direction of the weighted coefficients for PC1 and PC2. We see that coefficients for SAL.S and Secchi are a different sign from the others for PC1. Also, for PC2 water quality indicators (TURB.S, CHLA.S, TSS.S, TOC.S) have large positive coefficients compared to the negative coefficients for the nutrient levels (NH4, NO3, NOX, NO2, TKN, PO4, TP), SAL.S, and Secchi.

Cluster analysis of the ICAs and types.

We also used cluster analysis with Ward's method and present a dendrogram with similar broad conclusions (Fig. 7). The Inlet, Outfall and Reef sites are generally distinctive and form three main clusters. The Outfall sites are all quite similar to each other. The Reef sites are quite similar to each other, except Reef STL (which is more similar to JUP and STL Inlets). The Inlets BAK, BOC, HIL and BOY, GOC, PEV are fairly similar, but Inlet ILW is similar to Reefs.

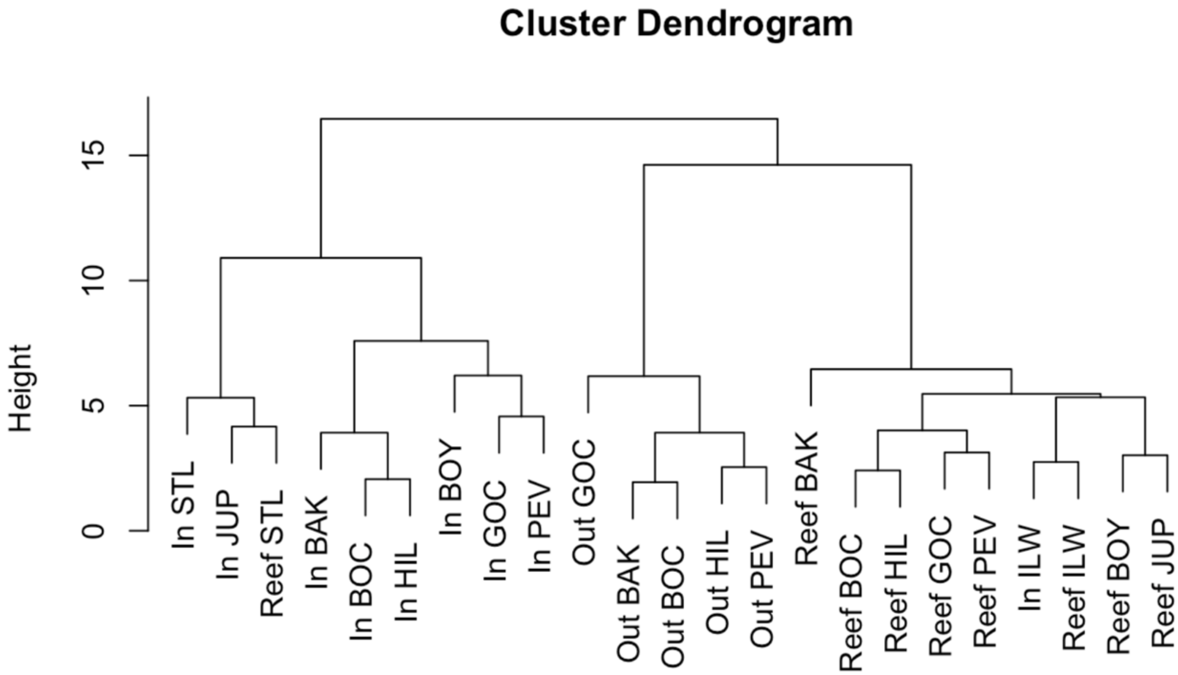


Figure 7. *Cluster analysis based on standardized logarithms of estimated upper quartiles. Ward's method is used for clustering.*

<u>Multidimensional Scaling</u>

An alternative method for dealing with the missing values is to carry out multidimensional scaling (MDS) on the Euclidean distance matrix between measures but omitting missing values. This results in similar plots as seen in PCA score plots. If there were no missing estimated quartiles the MDS and PCA score plots would be exactly the same, but it gives reassurance that two different methods of dealing with the missing values leads to the same conclusions about the sites and types. The PCA has the added bonus that interpretation of the relationships between the variables is possible.

Here we see that Figure 8 is very similar to Figure 2, so the use of MDS with omitting missing values and PCA with imputing missing values is very similar.

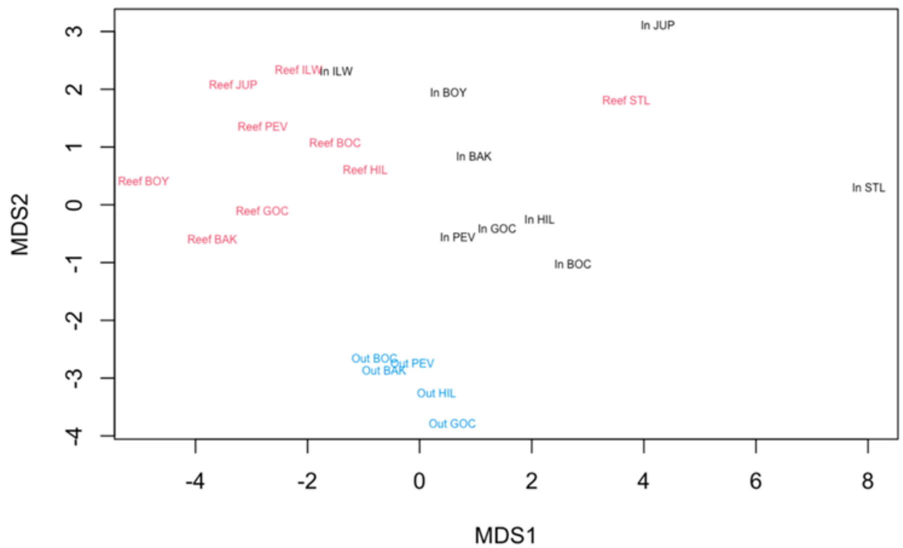


Figure 8: MDS using the standardized log estimated upper quartiles based on Euclidean distance, but removing missing values.

Additionally, we carried out paired t-tests between different types at ICAs. Readings are paired at the same site and at Surface/Bottom waters, thus aiming to account for the differences in ICAs and S/B. As previously we compared the estimated upper quartiles for each measure. A multiple comparisons adjustment is provided for carrying out multiple t tests using the Benjamini-Hochberg False Discovery Rate (Benjamini and Hochberg 1995).

Inlet versus Reef

	t	p	p-adjust
NH4	6.331	0	0
CHLA	7.298	0	0
NO3	2.449	0.025	0.029
NOX	2.945	0.009	0.013
NO2	3.728	0.002	0.004
TKN	5.511	0	0
PO4	3.375	0.005	0.008
TP	0.582	0.569	0.569
TSS	3.887	0.001	0.002
SAL	-2.557	0.02	0.025
SiO4	10.238	0	0
TOC	5.839	0	0
TURB	5.409	0	0
Secchi	-2.043	0.075	0.081

Table 5: Test for differences between Inlet vs Reef for the estimated upper quartiles. A positive t-statistic (t) means that the Inlet measurements are higher in value on average than the Reef values. The p-value (p) is from a paired t-test of no difference, and the p-adjust column is a multiple comparisons adjustment based on the Benjamini-Hochberg False Discovery Rate (FDR).

There is a significant difference in upper quartiles for all measures except TP and Secchi at the 5% level. The concentrations are all higher at Inlets except SAL which is lower. Secchi is significant at the 10% level, with Inlet having lower values than Reef. All except TP are significant using FDR=0.1 (the p-adjust column).

Reef versus Outfall

	t	p	p-adjust
NH4	-5.989	0.004	0.013
CHLA	3.932	0.017	0.037
NO3	-0.297	0.781	0.923
NOX	-10.084	0.001	0.007
NO2	-16.788	0	0
TKN	-2.161	0.097	0.14
PO4	-3.612	0.023	0.043
TP	-3.483	0.04	0.065
TSS	0.058	0.956	0.956
SiO4	-0.13	0.903	0.956
TOC	1.694	0.166	0.216
TURB	5.138	0.007	0.018
Secchi	-5.884	0.004	0.013

Table 6: *Test for differences between Reef vs Outfall for the estimated upper quartiles. A positive t-statistic means that the Reef measurements are higher in value on average than the Outfall values. The p-value is from a paired t-test of no difference, and the p-adjust is a multiple comparisons adjustment based on the Benjamini-Hochberg False Discovery Rate (FDR).*

Analytes NH4, NOX, NO2, PO4, TP and Secchi have significantly lower upper quartiles for Reef than Outfall. CHLA and TURB are significantly higher at Reef than Outfall (FDR=0.1).

Inlet versus Outfall

	t	p	p-adjust
NH4	-4.284	0.013	0.03
CHLA	5.259	0.006	0.021
NO3	2.204	0.092	0.143
NOX	-0.34	0.751	0.809
NO2	-5.457	0.005	0.021
TKN	-0.074	0.945	0.945
PO4	-1.45	0.243	0.284
TP	-3.144	0.035	0.061
TSS	1.441	0.223	0.284
SAL	-1.633	0.178	0.249
SiO4	4.825	0.008	0.022
TOC	3.189	0.033	0.061
TURB	13.989	0	0
Secchi	-11.189	0	0

Table 7: *Test for differences between Inlet vs Outfall for the estimated upper quartiles. A positive t-statistic means that the Inlet measurements are higher in value on average than the Outfall values. The p-value is from a paired t-test of no difference, and the p-adjust is a multiple comparisons adjustment based on the Benjamini-Hochberg False Discovery Rate (FDR).*

Analytes NH4, NO2, TP and Secchi have significantly lower upper quartiles for Inlet than Outfall. CHLA, SiO4, TOC, TURB are significantly higher at Inlet than Outfall. Here we use FDR=0.1.

<u>Summary</u>

Putting this all together we use > meaning significantly greater and < meaning significantly lower, and = not significantly different

NH4	Outfall > Inlet > Reef
CHLA	Inlet > Reef > Outfall
NO3	Inlet > Reef
NOX	Outfall = Inlet > Reef
NO2	Outfall > Inlet > Reef
TKN	Inlet > Reef
PO4	Outfall = Inlet > Reef
TP	Outfall > Inlet = Reef
TSS	Inlet > Reef
SAL	Reef > Inlet
SiO4	Inlet > Outfall = Reef
TOC	Inlet > Outfall = Reef
TURB	Inlet > Reef > Outfall
Secchi	Outfall > Reef > Inlet

Box-and-Whisker Plots

Typically, water quality data are skewed towards low concentrations and below detects resulting in non-normal distributions. Therefore, it is more appropriate to use the median as the measure of central tendency because the mean is inflated by high outliers. The box-and-whisker plot provides a powerful visualization of data distributions. The center horizontal line of the box is the median, the top and bottom of the box are the 25th and 75th percentiles (quartiles), and the ends of the whiskers are the 5th and 95th percentiles. The notch in the box bounds the 95% confidence interval of the median. When notches between boxes do not overlap, the medians may be considered significantly different. Outliers (<5th and >95th percentiles) were excluded from the graphs to reduce visual compression.

Inlets tend to show the highest variability in many WQ variables but not always the highest concentrations (Fig. 9&10). Outfalls tend to be highest in dissolved nutrients, with the exception of silicate. They also have good optical characteristics (turbidity, Secchi, and TSS) probably due to their large distance offshore. Reefs are generally low in nutrients with high quality optics.

One important characteristic to note is the difference between surface and bottom conditions among ICA types. Managers tend to characterize water quality using surface data, but it is the conditions at the bottom that may have most bearing on coral health. However, a recent study in the Florida Keys using regression trees showed that surface variables were more predictive of white pox disease at the bottom (Sutherland et al. 2023).

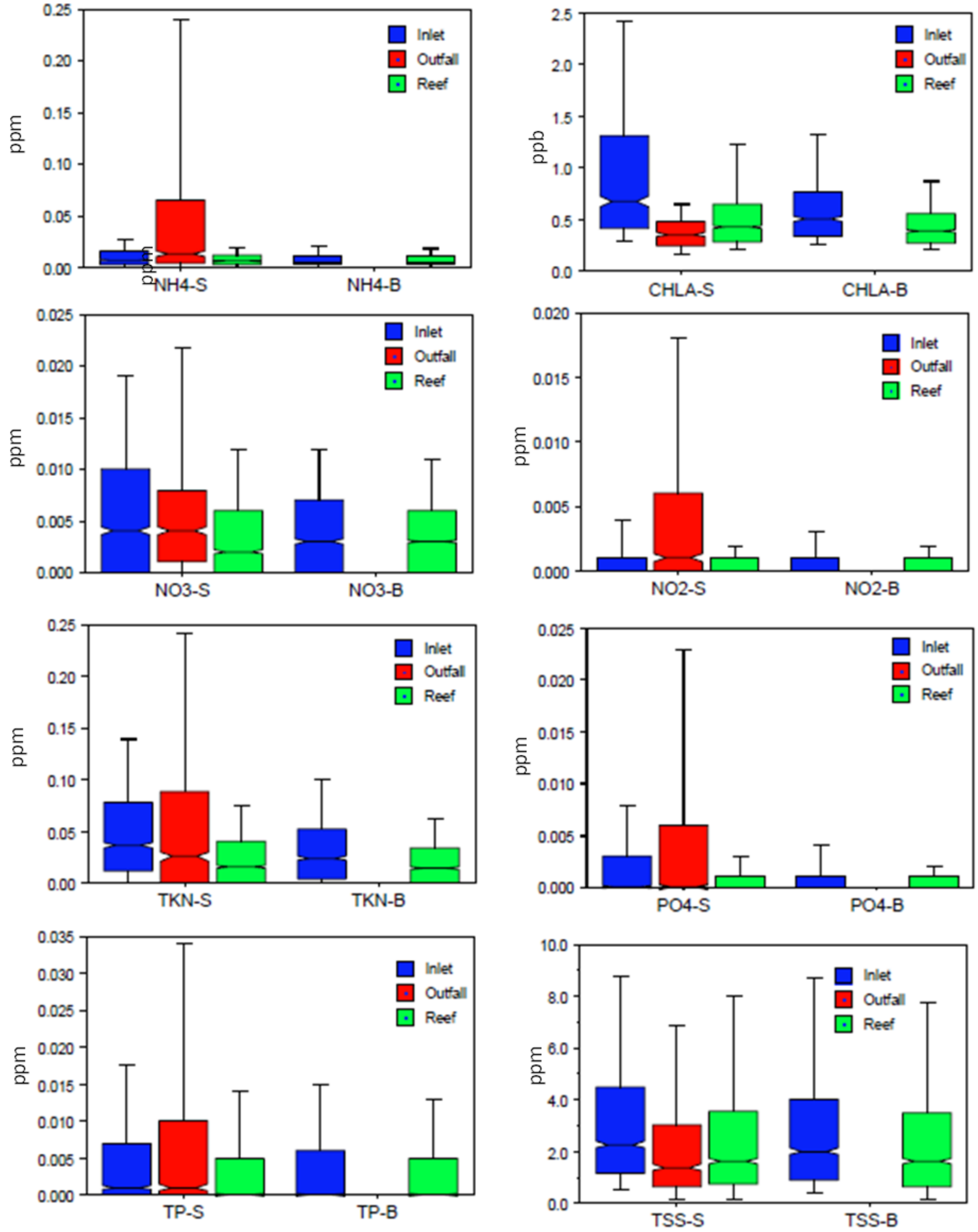


Figure 9. *Box-and-whisker plots for water quality variables by ICA Type and depth*

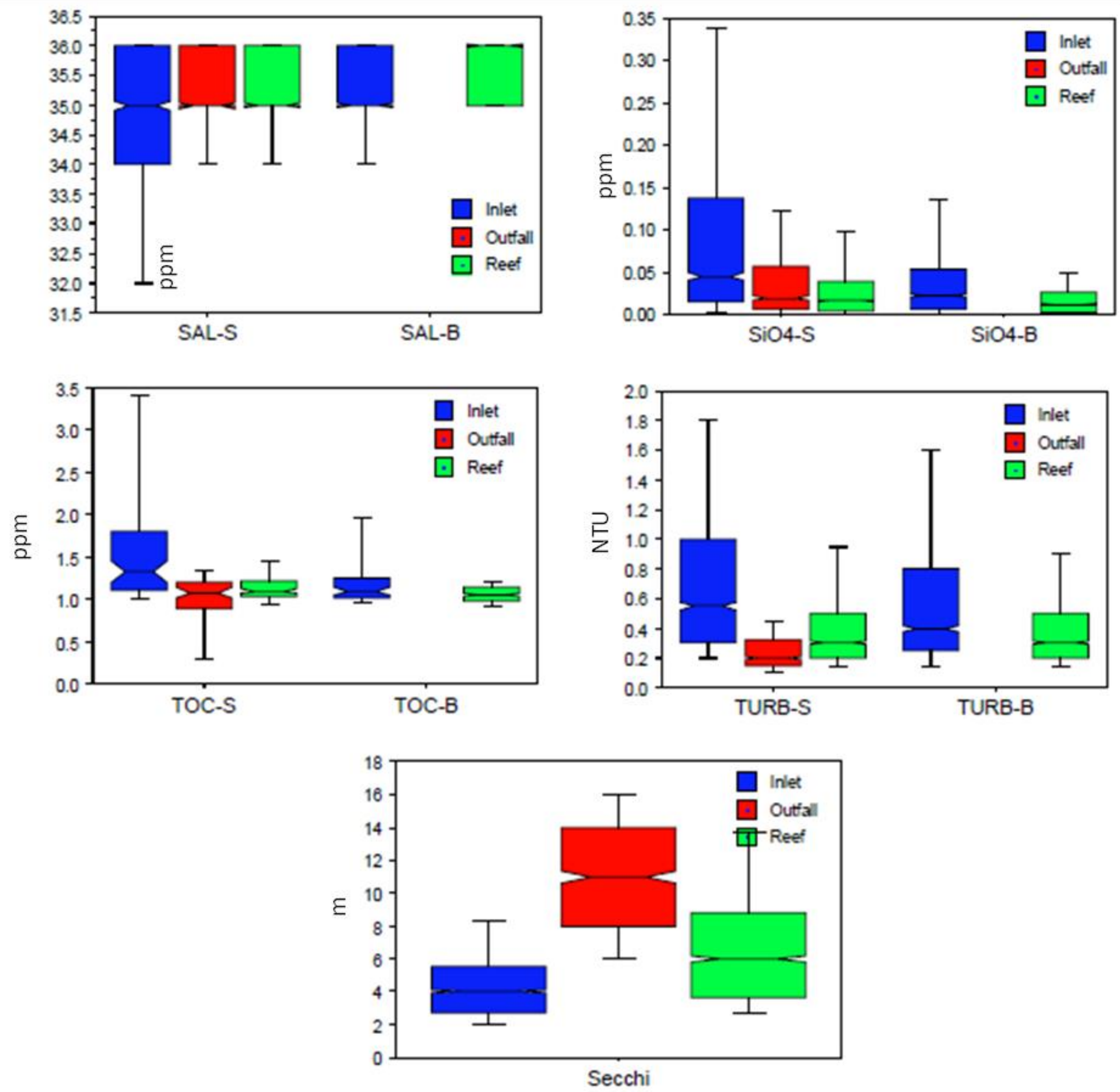


Figure 10. *Box-and-whisker plots for water quality variables by ICA Type and depth.*

Summary: Yes, water quality is different among "Site Types", but these categories have been subjectively applied to sampling sites. Objective analyses (PCA, MDS, and Cluster analysis) showed, with a few exceptions, that the classifications were distinct enough to be statistically different. Inlet sites all had similar water quality except for the STL, which was significantly different than other Inlets. The STL Reef sites clustered with other Inlet sites. Conversely, the ILW Inlet water quality clustered with other Reef sites. For future analyses, FDEP might want to reclassify some Site Types to be more consistent.

Does Water Quality Differ Between Surface and Bottom Waters?

To investigate the surface (S) versus bottom (B) variables we compared the estimated 75th percentiles for the variables, again using the estimated upper quartiles. We carried out paired t tests with pairing (S – B) at each ICA/type available. We give results for the Inlet ICAs and the Reef ICAs in Table 8. As there are only five Outfall ICAs with no bottom measurements we do not consider this type.

Inlet (S vs B)

	t	p	p-adjust
NH4	3.838	0.005	0.013
CHLA	4.354	0.002	0.009
NO3	1.899	0.094	0.1
NOX	2.596	0.032	0.046
NO2	3.468	0.008	0.015
TKN	3.716	0.006	0.013
PO4	4.764	0.005	0.013
TP	1.861	0.1	0.1
TSS	2.2	0.059	0.077
SAL	−3.162	0.013	0.021
SiO4	4.671	0.002	0.009
TOC	4.895	0.001	0.009
TURB	1.965	0.085	0.1

Table 8. *Test for differences between Surface and Bottom for the estimated upper quartiles of the Inlet sites. A positive t-statistic means that the Surface measurements are higher in value on average than the Bottom values. The p-value is from a paired t-test of no difference, and the p-adjust is a multiple comparisons adjustment based on the Benjamini-Hochberg False Discovery Rate (FDR).*

From Table 8 for the Inlet sites for all measures the upper quartiles are significantly higher at the Inlet Surface waters compared to Bottom waters, except for SAL which has lower values at the surface. In all cases there is significance at the 10% level and with multiple comparison adjustment using FDR=0.1.

Reef (S vs B)

	t	p	p-adjust
NH4	3.104	0.015	0.045
CHLA	3.642	0.007	0.042
NO3	-1.644	0.139	0.254
NOX	-1.104	0.302	0.453
NO2	1.603	0.148	0.254
TKN	2.267	0.053	0.127
PO4	0.794	0.453	0.557
TP	0.774	0.464	0.557
TSS	0.616	0.555	0.585
SiO4	3.779	0.005	0.042
TOC	3.072	0.015	0.045
TURB	-0.57	0.585	0.585

Table 9: *Test for differences between Surface and Bottom for the estimated upper quartiles of the Reef sites. A positive t-statistic means that the Surface measurements are higher in value on average than the Bottom values. The p-value is from a paired t-test of no difference, and the p-adjust is a multiple comparisons adjustment based on the Benjamini-Hochberg False Discovery Rate (FDR).*

From Table 9 there are significantly larger upper quartile values at the Reef surface vs bottom for NH_4, CHL*a*, SiO_4, TOC using p-value<0.1 or FDR<0.1, but no significant difference for NO_3, NOX, NO_2, TKN, PO_4, TP, TSS and TURB. For the Reef sites there are no differences in any values for SAL upper quartiles between surface and bottom and so the test cannot be carried out.

Summary: Yes, water quality is typically significantly different between surface and bottom samples from the same site. Variables most different tend to be those land-derived variables such as nutrients and sediments. These differences are complicated by current patterns and density stratification. Freshwater inputs from Inlets tend to remain at the surface rather than mix with depth. These areas also tend to have higher surface nutrient inputs. Outfall water sources enter at the bottom of the water column and are fresher than seawater. This means outfall sources tend to be buoyant and mix sewage nutrients throughout the water column.

TASK2: How Do Available Water Quality Data Compare to Relevant Published Benchmarks, Especially Those of SE Florida Waters?

The purpose of this Task is to provide a scientifically defensible methodology to ultimately assist FDEP in the development of biogeochemically relevant benchmarks for the Kristin Jacobs Coral Reef Ecosystem Conservation Area (ECA). Because of the diversity of South Florida's coastal areas regarding geomorphologic, climatic, circulation and ecosystem structure conditions coupled with differential human population distribution, intervention, and management activities, there is a general scientific consensus that uniform, region-wide benchmarks for coastal waters are not appropriate. As recommended by US-EPA (2001), biogeochemical benchmarks should be designed for specific waterbody types. Hence, we will attempt to derive benchmarks at the sub-basin level, called Inlet Contributing Areas (ICAs), using multiple approaches.

Presently, we do not know if the existing data is sufficient to develop those benchmarks for sustaining coral reef water quality. Therefore, we provided FDEP with comparisons of available ECA water quality data to relevant published data for coral reefs around the world, with special emphasis on Florida waters. This required a thorough literature search of peer-reviewed and grey literature. In addition, we attempted to develop benchmarks much like was done previously for South Florida coastal waters using a cumulative sum approach (Briceño et al. 2010).

In summary, a thorough literature search of peer-reviewed and grey literature was conducted. Existing ECA water quality concentrations were analyzed using EPA and FDEP approaches, and results presented by ICA. Comparison of ECA benchmarks to relevant published benchmarks for global coral reefs noting special conditions in southeast Florida were developed.

Task 2.1a: Discussion of Findings of Benchmarks for Coral Reef Waters

The development of water quality limits for coral reefs has been a long and difficult process. Not only are corals directly affected by nutrients, sediments, light field, etc. but they are also affected indirectly by changes wrought in the coral reef community e.g., algal overgrowth.

The scope of this bibliography is not to list the thousands of studies in the literature concerning the effects of nutrients on coral. Rather, we provide a compendium of those studies which strived to summarize these effects and draw a 'line in the water' by establishing water quality benchmarks to further the continued growth, development, and survival of coral reefs.

Early work in the 60's and 70's was mostly observational, much like Hart (1974). More refined empirical and nutrient dosing field studies provided the foundation for most governmental standards and criteria e.g., ANZECC, ARMCANZ (2000), GBRMPA (2009), FDEP (2013), Hawai'i State Department of Health (2021). Smith's pioneering work in Kaneohe Bay (1977) fired the starting gun for more in situ and lab-based studies.

For lab-based, experimental studies, the question has always been, which is the best measure to assess 'impact'? Some researchers have used rate of coral growth, some used mortality, and others used everything else in between. Bradley et al. (2010) provided a relevant discussion in relating the Clean Water Act to biocriteria as well as water quality criteria for coral reefs.

A recent meta-analysis on lab-based, experimental nutrient effects to corals by Nalley et al. (2023) attempted to address this multiple response problem by "classifying effects of DIN (nitrate and ammonium) and DIP (phosphate)" into nine physiological "coral holobiont responses":

A. Photosynthetic responses of the coral endosymbiont
    1. Zooxanthellae density
    2. Chl-*a* concentration
    3. Photosynthetic rate
    4. Photosynthetic efficiency (max. quantum yield)
B. Coral growth and calcification
    5. Growth rate
    6. Calcification rate
C. Mortality
    7. Adult tissue and colony survival
    8. Larval survival and settlement
    9. Fertilization success

The 10,911 studies initially identified were winnowed down to 395, then to 47 having "comparability among studies of response measurement units". These 47 studies focused on "manipulative experimental studies rather than observational …only 4 … were field studies".

Firstly, the authors' choice to limit experiments to use of inorganic nutrient forms downplays the role of organic N and P as nutrient sources. We know from many studies that DOP and DON typically constitute >80% of the ambient TN & TP pools (Jackson & Williams 1985, Karl et al. 1998, Briceño and Boyer 2020) and that they are readily bioavailable (P more so than N) (Berman & Bronk 2003, Boyer et al. 2006, Baldwin 2013, Jørgensen et al. 2014).

Secondly, the authors' exclusion of the many empirical and field-based studies negates decades of effort by the coral research community to develop consensus around nutrient effects on coral communities.

Thirdly, Nalley et al. (2023) reported large variability in benchmarks among the nine physiological responses, some having both negative and positive effects for the same nutrient. For example, higher nitrate concentrations increased photosynthetic responses but decreased coral growth and survival. Classifying these responses tended to reconcile some seemingly contradictory results in the literature, such as "Elevated nutrients may increase the abundance of zooxanthellae, positively affecting photosynthetic function, but beyond an optimal concentration … overcrowding may occur and lead to negative outcomes such as shading, increased holobiont temperature, and oxidative stress. In these cases, the addition of nutrients may result in a positive response up to a point, beyond which the response may become negative".

While this helps to untangle disparate nutrient responses, it makes it difficult for managers to integrate studies into benchmark development. It is also important to note that no one study measured nutrient responses to all nine physiological metrics. We believe that the value of the many empirical studies and field dosing experiments, being more inclusive of the coral community, should not be discounted and have therefore given more weight to this body of work for benchmark development. Further discussion of individual publications follows in **Task 2.1b** below.

Task 2.2: Coral Reef Water Quality Benchmark Setting Using Scientific Consensus

The following benchmark comparison (Table 10) was developed from references listed in Task 2.1 using our best knowledge and understanding of their content. The relevant chemical and physical variables are listed in columns across the top row with individual by reference in descending rows. In some instances, benchmarks consist of a range in values because the study may present multiple benchmarks for different geographical areas or coral physiological response. Note that we did not delve deeply into the effects of sedimentation and turbidity on coral because there is a separate FDEP project currently underway on that subject.

Our proposed Scientific Consensus of the published benchmarks described in Task 2.1b is summarized as follows:

- NH_4^+ 5 ppb
- NO_3^-+NO_2^- 5 ppb
- DIN 10 ppb
- PO_4^-/SRP 3 ppb
- TN 150 ppb
- TP 10 ppb
- Chl*a* 0.35-0.5 ppb
- Turbidity 0.5 NTU
- TSS 10 ppm
- Secchi 10 m
- K_d 0.14 m^{-1}

Reference	NH_4 (µg l^{-1})	NO_3+NO_2 (µg l^{-1})	DIN (µg l^{-1})	PO_4/SRP (µg l^{-1})	TN (µg l^{-1})	TP (µg l^{-1})	Chl*a* (µg l^{-1})	Turbidity (NTU)	TSS (mg l^{-1})	Secchi (m)	K_d (m^{-1})	Notes
ANZECC & ARMCANZ (2000)	1.0-10	1.0-8.0	2.0-18	2.0-5.0	100	10-15	0.5-1.4					GBR inshore & offshore
Bell & Tomascik (1993)							0.3					GBR
Bell (1992)			14	3.1-6.2			0.5					GBR
Boyer & Briceño (2010)	5.0	3.0	9.0	1.0	190	7.0	0.3	0.7			0.21	FKNMS 75th percentile
Briceño et al. (2010)					160	8.0	0.2					FKNMS - CUSUM analysis
De'ath & Fabricius (2008 & 2010)							0.3-0.6			10.0	0.14	GBR seasonal variations, 10 m Secchi ~ 0.144 Kd
Erftemeijer et al. (2012)								variable	10-**100**			very site specific
FDEP (2011)					142-162	6.2-7.1						Site-specific for FKNMS
FDEP (2013) Rule 62-302					170-250	7.0-11	0.3-0.7					Surface Water Quality Stds
FDEP (2021)								**4.5-7.0**				FL waters
FKRAD (2008)					125-**764**	7.0-13						multiple FKNMS zones
GBRMPA (2009)					20 (PN)	2.8 (PP)	0.45		2.0	10.0		gradient approach
Hawaii State DOH (2021)	2.0-3.5	3.5-5.0	5.5-8.5		110-150	16-20	0.15-0.30	0.2-0.5			0.1-0.2	open coastal waters
Hawker & Connell (1989)	**0.65**	1.3	2.0	**0.25**			0.59		3.9			Barbados applied to GBR
Houk et al. (2020)			(100-150)									Am. Samoa stream loading
Houk et al. (2022)			(100)									Guam stream loading
Japan Basic Environmental Law (1993)					200	20						Environ. Qual. Stds. for Coastal Waters
Koop et al. (2001)			**50**	6.2								ambient "control"
Lapointe (1997)			14	3.0								FKNMS
Moss et al. (2005)			1.0-5.0	3.0-8.0	120-155	12-20	0.3-0.6					GBR inshore & offshore
Nalley et al. (2023)			**140**	**9.3**								meta-analysis
Tomascik & Sander (1985)							0.4		4.0-5.0			GBR
Tuttle & Donahue (2022)									3.2-10			adult/juvenile
US-EPA Targets (2006, mod 2016)			10.5			7.7	0.35				0.20	FKNMS 75th percentile of baseline database

Table 10. *Scientific Consensus of coral reef water quality benchmarks.*

Benchmark Setting Using EPA 75th Percentile Approach

EPA recommends a reference site approach for setting benchmarks (US-EPA 2001) where sites are selected based on minimal human influence. If values from other sites fall within an acceptable range of reference sites (typically 75th percentile) they are considered to meet the designated use. In some areas minimally disturbed reference conditions no longer exist and may not be achievable. In these situations, "least disturbed sites" may be used (25th percentile) if they demonstrate that the existing biological community structure and function is representative of a sustainable, natural system. For comparative purposes, the 75th percentiles of relevant variables from each ICA are reported as well as the pooled values for the total ECA (Table 11). Note that ECA project reported TKN, not TN as previous studies, where TN = TKN + NO_3 + NO_2.

Bottom Samples	NH_4 (µg l^{-1})	NO_3+NO_2 (µg l^{-1})	DIN (µg l^{-1})	PO_4/SRP (µg l^{-1})	TN (µg l^{-1})	TP (µg l^{-1})	Chl*a* (µg l^{-1})	Turbidity (NTU)	TSS (mg l^{-1})	Secchi (m)	K_d (m^{-1})
All ECA	**13**	**8.0**	**21**	2.0	69	10	0.6	0.6		8.5	
BAK	**11**	**10**	**21**	0.0	51	4.0	0.7	0.7		7.6	
BOC	**11**	**8.0**	**19**	1.0	46	4.0	0.6	0.5		8.0	
BOY	**10**	**7.0**	**17**	0.0	35	3.0	0.5	0.4		**14.6**	
GOC	**22**	**8.0**	**30**	**12**	**246**	**27**	0.5	0.6		8.2	
HIL	8.0	**8.0**	**16**	1.0	46	4.0	0.7	0.5		8.5	
ILW	**9.0**	6.0	15	1.0	42	4.0	0.5	0.5		6.9	
JUP	**12**	**7.0**	**19**	1.0	50	6.0	0.7	0.9		**11.0**	
PEV	8.0	6.0	14	0.0	35	6.0	0.5	0.4		9.0	
STL	**22**	9.0	**31**	**14**	**292**	**36**	**1.2**	**2.1**		4.0	

Table 11. *75th percentiles of relevant variables from each ICA and pooled values for the total ECA.*

Benchmark Setting Using CUSUM Approach

An ecological threshold is the critical value of an environmental driver for which small changes can produce an abrupt shift in ecosystem conditions, where core ecosystem functions, structures and processes are essentially changed between alternative states (Andersen et al. 2008). The following section describes our approach to characterize abrupt changes (benchmarks) of selected ecological system-response indicators (Boyer et al. 2009) as potential drivers change their magnitude.

The method is quite simple but robust (Briceño et al 2010; Regier et al. 2019) and entails calculating and plotting a cumulative sum of standardized response values along the corresponding driver's gradient. The benchmark location is highlighted by a sharp and sustained turn from below (above) average response concentration to above (below) average response concentrations. In order to calculate the cumulative sum of standardized response values (z_i), we apply equation (1) to the response (x_i) data, ordered by the driver's level. Therefore, a direct driver:response relationship will render a V shape line-plot, while an inverse driver:response relationship will generate a peak-shaped curve (Fig 11).

$$z_i = [(x_i - m)/\sigma] + z_{i-1} \qquad (1)$$

where m=mean and σ=standard deviation.

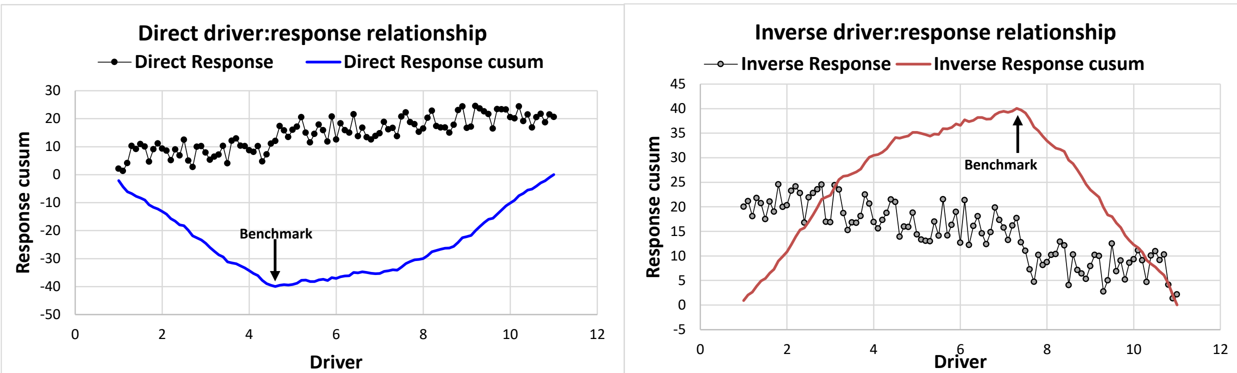


__Figure 11.__ Left: Monotonically increasing trend in the dataset renders a V-shaped CUSUM plot; Right: Monotonically declining trend in the dataset renders a peak-shaped CUSUM plot. Also shown are the location of benchmarks

The CUSUM methodology is very robust against data gaps and provides a good approximation of the real time-series tendency, even when gaps amount up to 80% of the original data set (Regier et al. 2019), as shown in Figure 12. Nevertheless, if the gaps are not random but preferentially concentrated on a portion of the time series, as we observe in the ECA data (Table 2), results are not as good.

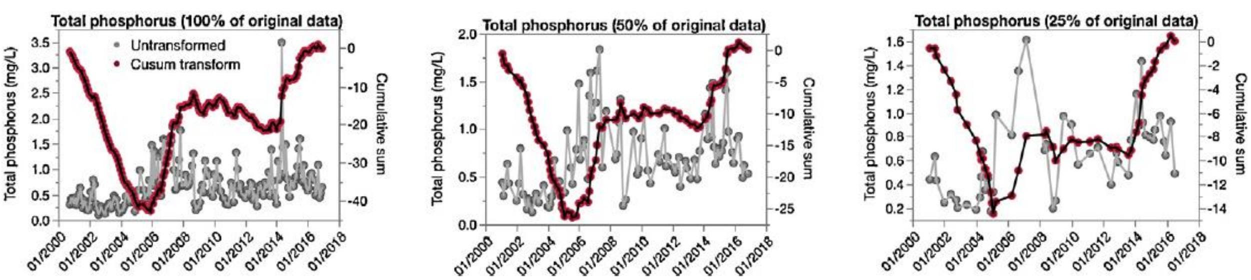


__Figure 12.__ Cumulative sums calculated from a total phosphorus time-series (left), and with 50% (center) and 75% (right) of the points randomly removed from the timeseries to demonstrate cumulative sums as a method robust to data gaps. From Regier et al. 2019.

Considering the robustness of the CUSUM approach to data gaps we tried the construction of these CUSUM charts with ECA dummy-free data, but the resulting thresholds were too biased towards high values, because the gaps were concentrated on the lower end of the data series. We have confronted this issue in the past and by testing artificial time series and selected thresholds, we found that the threshold would not change as far as the highest detection limit in the gap-free data is below the original threshold. Given that we do not know the real thresholds for the study area, we can only predict that if the number of censored values is more than 50% of the dataset, meaning the maximum DL is above the original median of the dataset, the resulting threshold will be biased. As shown in Table 2, most of the ECA data is beyond that 50% level.

Benchmark Derivation Using CUSUM of SEFCRI Data

During the development of a Local Action Strategy (LAS) targeting four threat areas as the focus for immediate action to protect the reefs of southeast Florida a preliminary monitoring program was implemented in southeast Florida coral reefs. That program was named, the Southeast Florida Coral Reef Initiative (SEFCRI; Boyer et al. 2011), whose objective was to establish a long-term offshore water quality monitoring program along the coral reef ecosystems in Miami-Dade, Broward, Palm Beach, and Martin counties – collectively, the southeast Florida region (Fig 13). That program became the Kristin Jacobs Coral Reef Ecosystem Conservation Area (Coral ECA) Water Quality Assessment (WQA) in 2014. ECA sampling sites were not co-located with the SEFCRI sites, but hopefully these older data would provide an approximate picture of water quality in the region.

The period of record (POR) for this program was from 12/8/2009 to 9/7/2012, and the measured physicochemical parameters included depth (m), salinity (PSU), temperature (°C), dissolved oxygen (DO in mg l^{-1}), turbidity (NTU), and PAR ($\mu E\ m^{-2}\ s^{-1}$). The light extinction coefficient (K_d in m^{-1}) was calculated as a log function from PAR measurements through the water column. The laboratory analyses included dissolved ammonium (NH_4^+), dissolved nitrate + nitrite (N+N), dissolved nitrite (NO_2^-), soluble reactive phosphate (SRP), total nitrogen (TN), total phosphorus (TP), total organic carbon (TOC), and total silicate (SiO_2). The biological parameter was chlorophyll a (CHLA). Some parameters were not measured directly but calculated by difference. Dissolved nitrate (NO_3^-) calculated as N+N – NO_2^-; dissolved inorganic nitrogen (DIN) calculated as N+N + NH_4^+. Total organic nitrogen (TON) was defined as TN - DIN. Data is shown in file **SEFCRI-FIU Database.xlsx**

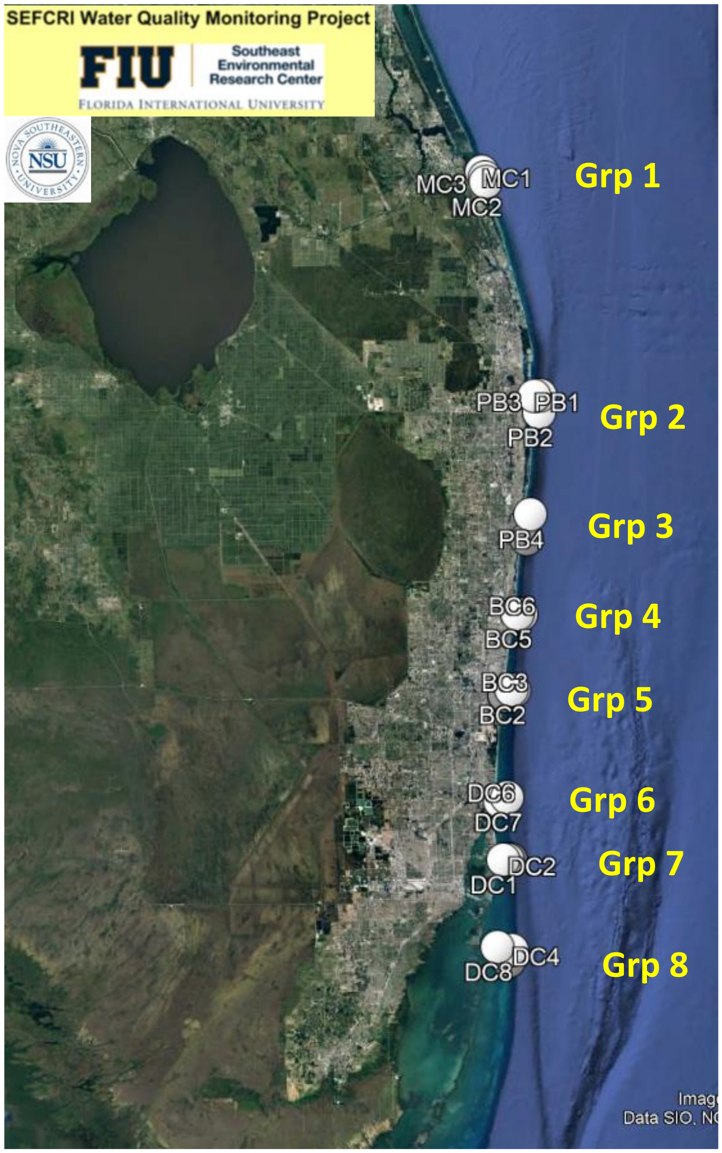


Figure 13. *Southeast Florida Coral Reef Initiative (SEFCRI) spatial domain, showing sampling sites in Miami-Dade, Broward, Palm Beach, and Martin County. Groups of closely located samples (Grp 1 to 8) were used for cluster analysis.*

Results from cusum analysis improve with the volume of data, and given the short POR for the SEFCRI effort, we tried to combine enough data to run the CUSUM analyses. Similar grouping approach was successfully applied when classifying south Florida coastal waters, which rendered support to the designation of water quality criteria by EPA-FDEP (Briceño et al. 2013). First, we designed 8 groups of closely spaced sampling sites as shown in Figure 13. Then, we performed a Cluster Analysis (MINITAB 16®) of the Groups of sampling sites. Results are presented in Table 11 and the dendrogram of Figure 14. Stations were clustered as shown in Table 12. These clusters are both spatially associated (groups) and biogeochemically linked clustering with similarity level > 98%. Detail of what station belongs to each group and each cluster is shown in Table 12.

Cluster Analysis of Variables: GRP1. GRP2. GRP3. GRP4. GRP5. GRP6. GRP7, GRP8

Correlation Coefficient Distance, Complete Linkage

Amalgamation Steps

Step	Number of clusters	Similarity level	Distance level	Clusters joined		New cluster	Number of obs. in new cluster
1	7	99.9959	0.0000817	3	4	3	2
2	6	99.9873	0.0002541	1	7	1	2
3	5	99.9841	0.0003189	3	6	3	3
4	4	99.9835	0.0003292	2	8	2	2
5	3	99.9181	0.0016373	1	2	1	4
6	2	99.8701	0.0025982	1	5	1	5
7	1	98.9434	0.0211324	1	3	1	8

Final Partition

	Variables		
Cluster 1	GRP1	GRP7	
Cluster 2	GRP2	GRP8	
Cluster 3	GRP3	GRP4	GRP6
Cluster 4	GRP5		

Table 11. *Results of Cluster Analysis of SEFCRI water quality data*

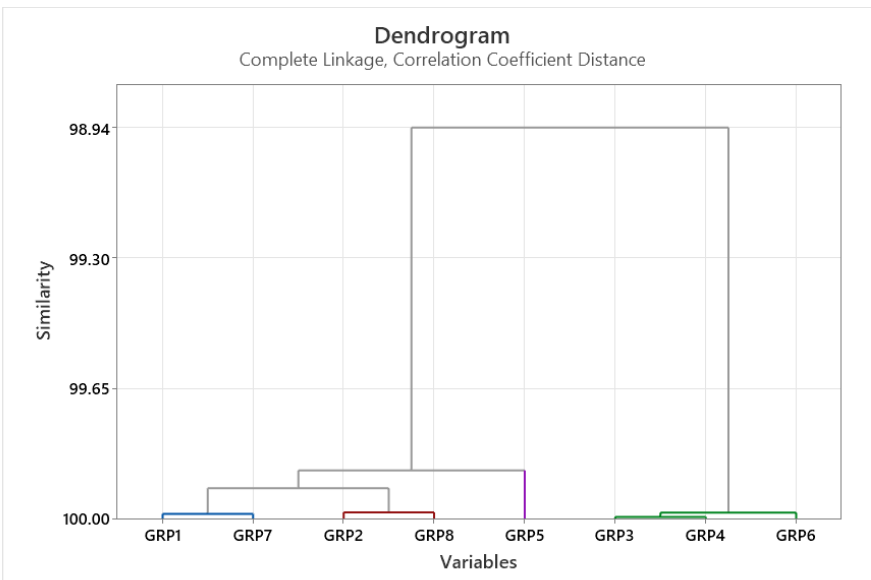


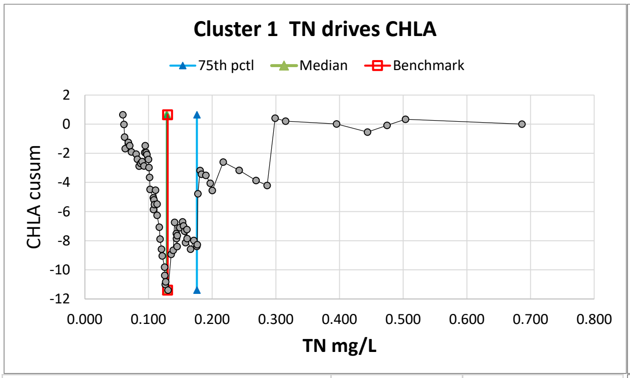
Figure 14. *Dendrogram for clustering of sampling Groups shown in Figure 13. Similarity level >99.8*

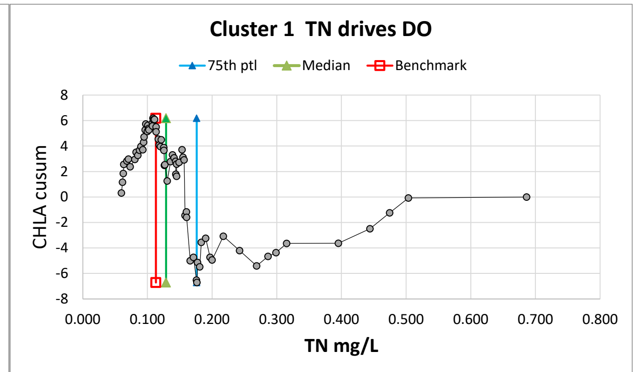
Cluster	Group	Stations
Cluster 1	Group 1	MC1, MC2, MC3
	Group 7	DC1, DC2, DC3
Cluster 2	Group 2	PB1, PB2, PB3
	Group 8	DC4, DC5, DC8
Cluster 3	Group 3	PB4, PB5
	Group 4	BC5, BC6
	Group 6	DC6, DC7
Cluster 4	Gropu5	BC1, BC2, BC3, BCA

Table 12. *Content of each cluster in terms of groups and stations*

In order to assess how the water system reacts to increasing level of drivers of change, we selected the three variables as system responses (CHL*a*, DO and K_d), and seven variables as drivers of change (TN, TIN, TP, SRP, TURB, NH4 and NOX). In other words, we will attempt to discern how the response variables react to changes in driver's magnitude. Conceptually it is similar to analyze results of a nutrient dose experiment. The driver-response plot is constructed using two variables with paired observations, one that is a potential driver (e.g. nutrient concentration, water turbidity etc.), and the other a potential response. First, the paired measurements are ordered so the driver variable is organized in ascending order. The reordered response variable is then CUSUM-transformed following Eq. (1). Figures 15 to 18 show examples of these plots and the data gathered from them.

As seen in the example of Figure 15, the driver's (TN) concentration at which the line-plot changes from steep negative slope (mostly below average CHL*a*) to steep positive slope (mostly above average CHL*a*), marks the TN benchmark for Cluster 1. Likewise, the average concentration of CHL*a* for samples below the TN benchmark are the benchmark CHL*a* concentration for that driver at that Cluster. Similar approach is followed for TN benchmarks for DO and Kd. In total, we constructed 84 Driver : Response diagrams like the ones in figures 15 to 18 for the whole dataset and derived the corresponding benchmarks. Results are shown in Table 13





	Benchmark	Below Bench
Cluster 1 TN drives CHLA	0.130	0.4092
Cluster 1 TN drives DO	0.113	6.6604
Cluster 1 TN drives Kd	0.157	0.1193

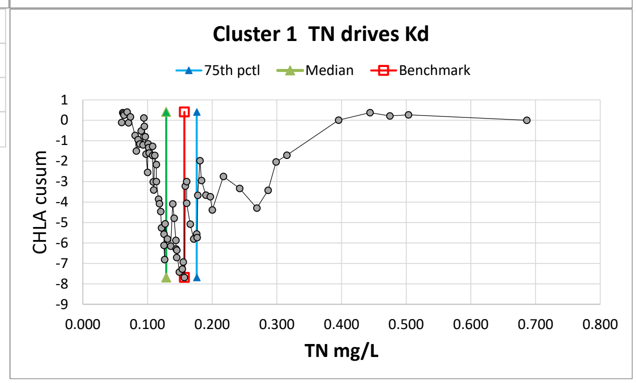
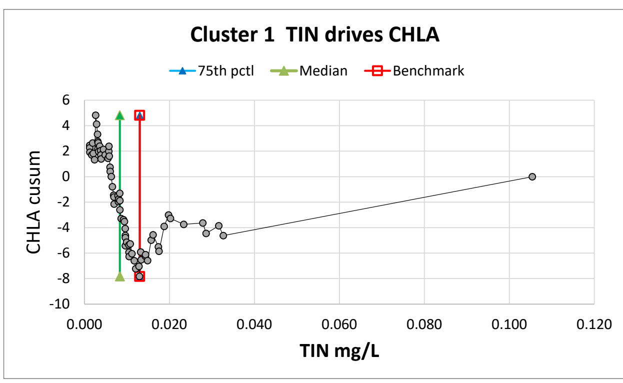
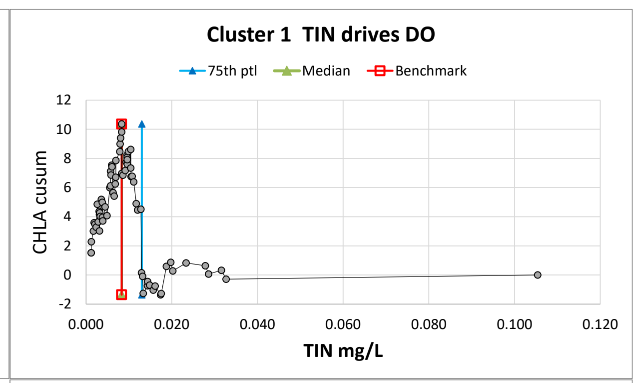


Figure 15. *Driver (TN): Response (CHLa, DO and K_d) diagrams for sites in Cluster 1. The red vertical line shows the location of the TN benchmark. Below Bench is the average concentration of the response variable for samples below the benchmark*





	Benchmark	Below Bench
Cluster 1 TIN drives CHLA	0.013	0.4813
Cluster 1 TIN drives DO	0.0083	6.6797
Cluster 1 TIN drives Kd	0.012	0.1168

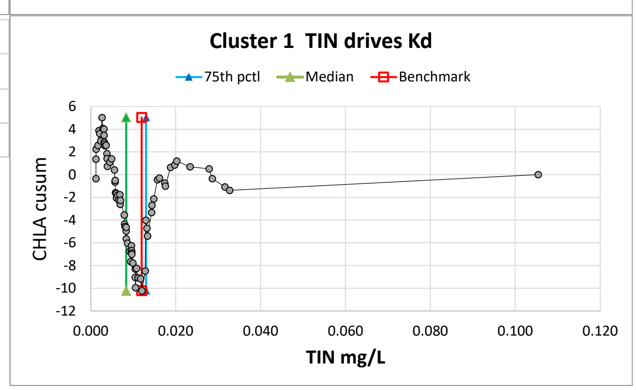
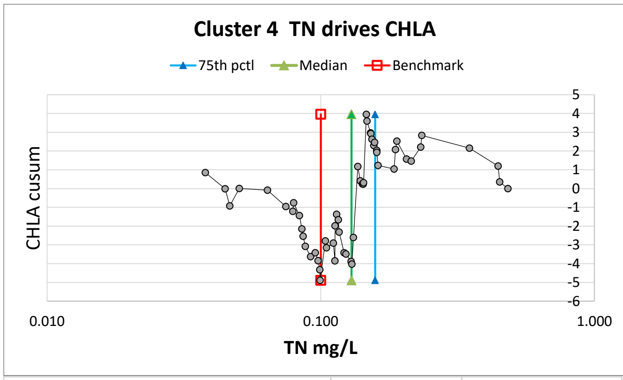
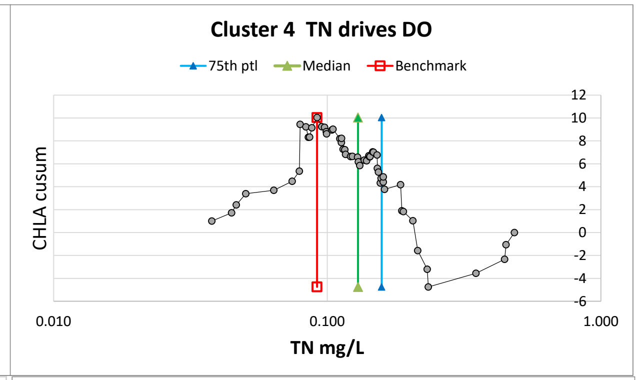


Figure 16. *Driver (TIN): Response (CHLa, DO and K_d) diagrams for sites in Cluster 1.*





	Benchmark	Below Bench
Cluster 4 TN drives CHLA	0.1000	0.3867
Cluster 4 TN drives DO	0.0918	6.9053
Cluster 4 TN drives Kd	0.1619	0.1531

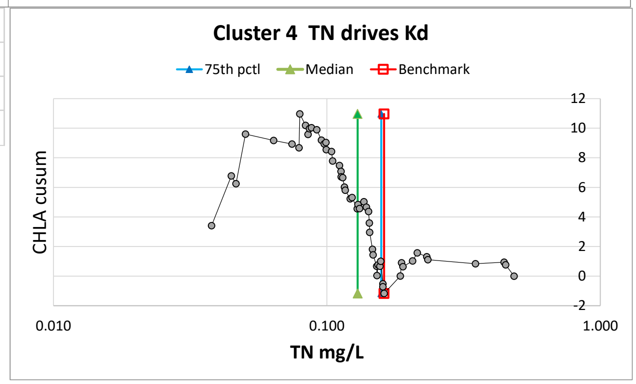
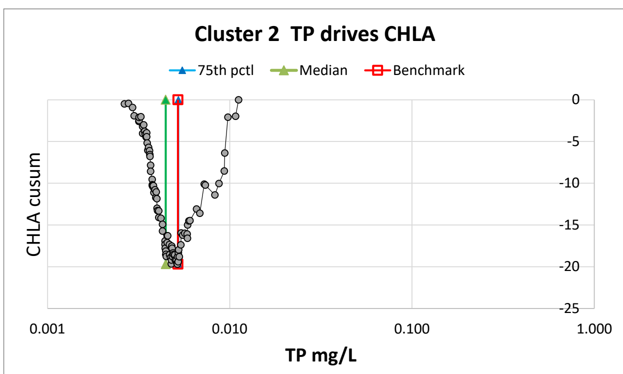
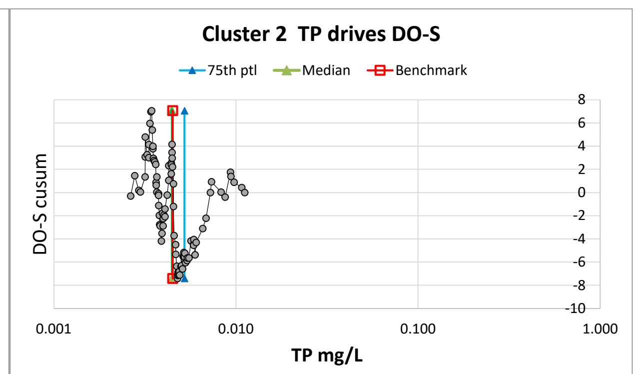


Figure 17. *Driver (TN): Response (CHLa, DO and K_d) diagrams for sites in Cluster 1*





	Benchmark	Below Bench
Cluster 2 TP drives CHLA	0.0052	0.2973
Cluster 2 TP drives DO-S	0.0045	6.5446
Cluster 2 TP drives Kd	0.0059	0.0674

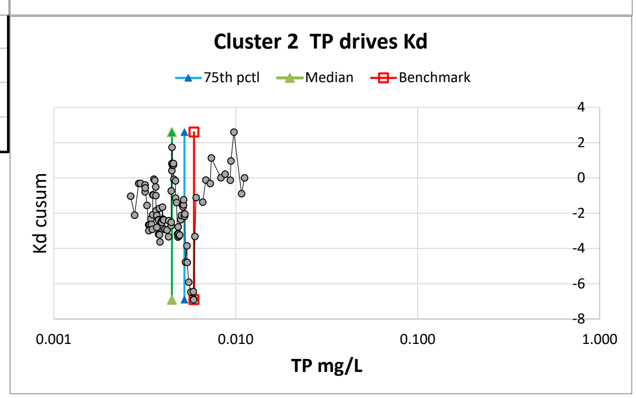


Figure 18. *Driver (TP): Response (CHLa, DO and K_d) diagrams for sites in Cluster 2*

.

	Cluster 1		Cluster 2		Cluster 3		Cluster 4	
Driver	Benchmark	Below Bench	Benchmark	Below Bench	Benchmark	Below Bench	Benchmark	Below Bench
TN drives CHLA	0.130	0.409	0.105	0.276	0.098	0.507	0.100	0.387
TN drives DO-S	0.113	6.660	0.081	6.744	0.090	6.651	0.092	6.905
TN drives Kd	0.157	0.119	0.103	0.073	0.105	0.086	0.162	0.153
TIN drives CHLA	0.013	0.481	0.010	0.359	NA	NA	0.009	0.420
TIN drives DO-S	0.008	6.680	0.006	6.555	0.009	6.609	0.005	6.322
TIN drives Kd	0.012	0.117	0.008	0.066	0.008	0.087	0.010	0.121
TP drives CHLA	0.006	0.340	0.005	0.297	0.007	0.444	0.006	0.360
TP drives DO-S	NA	NA	0.005	6.545	0.006	6.591	0.006	6.606
TP drives Kd	0.006	0.090	0.006	0.067	0.006	0.086	0.005	0.123
SRP drives CHLA	0.002	0.474	NA	NA	NA	NA	0.001	0.489
SRP drives DO-S	NA	NA	0.001	6.549	NA	NA	0.001	6.555
SRP drives Kd	0.002	0.121	NA	NA	0.001	0.092	0.001	0.136
TURB drives CHLA	0.350	0.369	0.200	0.340	0.010	0.412	0.200	0.356
TURB drives DO-S	NA	NA	0.100	6.547	0.080	6.612	0.700	6.579
TURB drives Kd	0.521	0.121	0.120	0.060	0.300	0.087	0.700	0.110
NH4 drives CHLA	0.008	0.500	0.002	0.424	NA	NA	0.004	0.448
NH4 drives DO-S	0.007	6.599	NA	NA	0.004	6.601	0.006	6.603
NH4 drives Kd	0.006	0.120	0.002	0.054	NA	NA	0.003	0.131
NOX drives CHLA	0.003	0.492	0.002	0.307	NA	NA	0.003	0.479
NOX drives DO-S	0.003	6.613	0.001	6.663	0.004	6.614	0.014	6.584
NOX drives Kd	0.005	0.132	0.002	0.067	0.003	NA	0.003	0.121

Table 13. *Benchmarks for drivers (TN, TIN, TP, SRP, TURB, NH_4 and NO_X) and system responses (CHLA, DO and K_d).*

TN benchmarks are very similar (mean= 111 ug/L; σ=17 ug/L; COV=16%), as are TIN (mean=9 ug/L; σ=1ug/L; COV=19%), TP (mean=6 ug/L; σ=0.4 ug/L; COV=8%), CHLa (mean=0.41 ug/L; σ=0.005 ug/L; COV=13%), and DO (mean=90 ug/L; σ=19 ug/L; COV=0.3%) benchmarks. On the other hand, Kd (mean=0.09 m^{-1}; σ=0.02 m^{-1}; COV=29%), SRP (mean=2 ug/L; σ=0.4 ug/L; COV=32%), NOX (mean=4 ug/L; COV=48%), NH4 (mean= 4 ug/L; σ=2 ug/L), and especially Turbidity (mean=0.31 NTU; σ=0.20 NTU; COV=48%) are more varied.

The location of a given benchmark with respect to the median concentration of the driver is of special interest. If the benchmark coincides with the median, small increases in the driver concentration may cascade into disturbed conditions, where the response is either an algal bloom (high CHL*a*), anoxia (low DO) or low light penetration (hi K_d). If the benchmark is below the median, the system is disturbed, because it is kept most of the time (more than 50% of the time) with excess concentrations of the driver, like for TN as driver of CHLa and DO for Cluster 4, shown in Figure 17. Finally, a system where the driver's benchmark is above the median is probably a healthy system with respect to the impacts of that driver.

Results from the CUSUM analysis of SEFCRI data indicate that benchmarks for the following drivers are below the median of the driver variables as shown in Table 14. Therefore, the most common problematic driver is TN and the most common response from the system to high TN concentrations is DO, followed by CHL*a*. Likewise, the most affected cluster, where more drivers have benchmarks below the mean, is Cluster 4, followed by Cluster 2.

Cluster	Driver	Below median of
Cluster 1	TN	DO
Cluster 2	TN	CHLa, DO, Kd
	NH4	CHLa, Kd
	NOX	DO
Cluster 3	TN	DO
Cluster 4	TN	CHLa, DO
	TIN	DO
	TP	Kd
	SRP	CHLa, DO
	NH4	Kd

Table 14. *Benchmarks for drivers below the median of response variables.*

Benchmark Approach Comparison

The three separate benchmark approaches are compared in Table 12. The 75th percentiles for total ECA compare relatively well with Scientific Consensus benchmarks, DIN values were higher in the ECA than proposed and Secchi depth was lower. The CUSUM benchmarks (CHL*a* response variable) vary by Site Types. Overall, CUSUM Reef benchmarks for most nutrients were lower than the other approaches.

Variable	Consensus	75th percentile	Cluster 1	Cluster 2	Cluster 3	Cluster 4
$NH4^{+}$ (ppb)	**5**	**13**	7	2	4	4
$NO3^{-}$ + $NO2^{-}$ (ppb)	**5**	**8**	4	2	4	7
DIN (ppb)	**10**	**21**	11	8	9	8
$PO4^{-}$ (ppb)	**3**	**2**	2	1	1	1
TN (ppb)	**150**	**69**	133	96	97	118
TP (ppb)	**10**	**10**	6	5	6	5
CHLa (µg)	**0.3-0.5**	**0.6**	0.4	0.3	0.5	0.4
Turbidity (NTU)	**0.5**	**0.6**	0.4	0.1	0.1	0.5
TSS (ppm)	**10**		a	a	a	a
Secchi (m)	**10**	**8.5**	a	a	a	a
Kd (m^{-1})	**0.14**		0.12	0.06	0.09	0.13

Table 15. *Three separate benchmark approaches for ECA.*

Recommendations

We have three general recommendations concerning this project moving forward. The first reiterates a recommendation from our previous report (Briceño et al. 2022) that FDEP should work to reduce the number of non-detects in future laboratory analyses. This means either upgrading the existing laboratory sensitivity for low level nutrient analyses or by using a different contract laboratory with higher analytic sensitivity.

The second recommendation concerns treatment of non-detect data. Censored maximum likelihood estimation is an efficient method to estimate the distributions, taking account of the observations below the MDL. If more readings can be obtained over the MDL then different estimation methods will become more similar, and ideally the analysis should not be very sensitive to the choice of estimation method.

The third recommendation concerns derivation of water quality benchmarks. Each approach, the Scientific Consensus, 75th Percentile, and CUSUM, are valid methods in their own right. Surprisingly, the results of all three approaches for the ECA water quality were similar for NO_3+NO_2, PO_4, CHL*a*, turbidity, and Secchi depth. The Scientific Consensus result was lower for NH_4 but higher than the other two approaches for TN.

We believe that the choice of which benchmark approach to use for the ECA should be debated by the local coral reef scientific and regulatory community. There are advantages and disadvantages for each method. Advantages of the Scientific Consensus are that there is considerable weight of evidence generated from the many peer-reviewed studies and that these results all fall within a relatively narrow range. The disadvantages include inherent variability in laboratory analyses, fluctuations in geographical ambient nutrient levels, global differences in coral community structure, etc.

An advantage of the 75th Percentile approach is that it uses data generated from the local area of interest. It may also be used to mine historical data. Conversely, the main disadvantage of the 75th Percentile approach is that it relies on data collected from the local area of interest. If the area of interest is already impacted, the benchmarks will be overestimated. However, future benchmarking could be refined by more selective use of least-impacted ICAs. The PC/MDS/Cluster analyses showed that data from most Inlets should be excluded from the computation because they are very different than Reef sites. Conversely, the ILW might be included in REEF as its water quality was comparable with other Reef sites. Outfall sites are problematic because they typically occur farther from shore and in deeper waters than Reefs (2.1-17.1 m vs 16.8-54.9 m). In addition, there is no data collected at bottom Outfall sites where impacts may be expected.

The CUSUM approach also relies on local data but has the advantage that it quantifies a driver-response benchmark for increase in CHL*a* production (phytoplankton biomass), decline in DO or decline in water transparency (Kd). The disadvantage is that, currently, there are no other driver-response effects in place for coral reef impacts which occur at the same time scale of water quality sampling events. Lags between driver-response reduce the ability to resolve thresholds.

Task 2.1b: Annotated Bibliography of Benchmarks for Coral Reef Waters

1) ANZECC, ARMCANZ (2000) Australian and New Zealand Guidelines for Fresh and Marine Water Quality. Australian and New Zealand Environment Conservation Council and Agriculture and Resource Management Council of Australian and New Zealand, Canberra.

This document combines Australian and New Zealand government determinations of nutrient criteria for the water of the Great Barrier Reef. It has been updated and hosted online as the Australian & New Zealand Guidelines for Fresh & Marine Water Quality https://www.waterquality.gov.au/anz-guidelines. See GBRMPA (2009) for more details.

> *"It is important to know that the Water Quality Guidelines' DGVs [Default Guideline Values] are not mandatory and have no formal legal status, but that, where appropriate, state, territory or local jurisdictions may incorporate the processes and tools, including the DGVs, provided within the Water Quality Guidelines, into their water quality protection policy and regulatory tools."*

> *"Ideally, use guideline values with measurements from other lines of evidence in a weight-of-evidence process to determine if water quality represents a risk to a particular community value."*

2) Bell PRF (1992) Eutrophication and coral reefs - some examples in the Great Barrier Reef Lagoon. *Water Res* 26:553–568.

This paper summarizes data from a systematic study of nutrient concentrations from the GBR lagoon and compares them with those found for other coral reef regions. It also discusses and suggests eutrophication benchmarks for coral reefs.

> *"Chlorophyll a appears to be the best water quality indicator of eutrophication in coral reef regions and a eutrophication benchmark value (annual mean) at or below 0.5 mg m^3 [0.5 ppb] is suggested. The concentrations of nutrients N and P associated with the onset eutrophication in coral reef communities are less well defined (annual mean DIN ~1 µM [14 ppb]; P-PO_4 ~ 0.1-0.2 µM [3.1-6.2 ppb]) but are in accord with [other] eutrophication benchmark levels".*

3) **Bell PRF, Tomascik T (1993) The demise of the fringing coral reefs of Barbados and regions in the Great Barrier Reef (GBR) lagoon-impacts of eutrophication. In: Proceedings of the Colloquium on Global Aspects of Coral Reefs - Health, Hazards, and History. Ginsburg RN (ed). University of Miami, Miami, pp. 319–325.**

A reassessment of the benchmarks published in Bell et al. (1992) in which they suggest lowering the chlorophyll *a* benchmark to 0.3 ppb.

> *"The nutrient benchmark concentrations are of the same order as the half-saturation constants of many marine phytoplankton (and probably attached algae) and hence variations around these concentrations will significantly affect the rate of growth of the algae and hence affect the ability of the algae to compete with the corals."*

> *"A closer examination of the historical data for Barbados is presented below and this indicates that an even lower benchmark level is appropriate for that region and possibly the Caribbean as a whole … A value of 0.3 mg chlorophyll a m^{-3} is chosen. This benchmark concentration may appear low but is in fact twice the open water background level."*

4) **Boyer JN, Briceño H (2010) Nutrient criteria in the Florida Keys National Marine Sanctuary and Dry Tortugas National Park. Presented at the FDEP Estuary and Coastal Numeric Nutrient Criteria Development Meeting, Miami, FL, March 3, 2010.**

Presented to the FDEP MTAC during the process of developing numeric nutrient criteria for South Florida waters. Results of FIU data analysis from 15 years of quarterly sampling at ~150 sites in the FKNMS using EPA 75^{th} percentile approach. The main caveat to using this method is the assumption that ambient conditions are reasonably protective (see Bradley et al. 2009 for further discussion). This seems to be the case for the FKNMS as the proposed benchmarks are comparable to other assessments.

5) **Briceño H, Boyer JN, Harlem P (2010) Proposed methodology for the assessment of protective numeric nutrient criteria for South Florida estuaries and coastal waters. Submitted to the EPA Science Advisory Board (SAB).**

The EPA Science Advisory Board reviewed proposed numeric nutrient criteria for Florida and solicited comments. This whitepaper response described a statistical method using CUSUM analysis to develop biologically-relevant benchmarks as numeric nutrient criteria for South Florida coastal region. The same recommendations were submitted to FDEP MTAC. Ultimately many of the recommendations were adopted into Florida Rules, Chapter 62-302, Surface Water Quality Standards (see FDEP (2013))

6) **De'ath G, Fabricius K (2010) Water quality as a regional driver of coral biodiversity and macroalgae on the Great Barrier Reef. *Ecolog Appl* 20:840–850.**

A peer-reviewed publication of De'ath and Fabricius (2008) report which describes "trigger values" of Chl *a* and Secchi depth for the GBR. They used the unaltered Cape York region as a reference location for setting limits.

> *"Choosing the Cape York values and the means of the ranges in the response curves, we postulate that the ecological condition of the GBR would significantly higher if mean annual water clarity does not drop below 10 m Secchi depth (at shallower depths Secchi will be visible on the seafloor) and mean annual chlorophyll concentration remains below 0.45 μg L^{-1}. These values should become the guideline triggers for water quality management. Further reductions in chlorophyll and increases in water clarity would provide additional significant improvement in ecosystem status."*

7) **Erftemeijer PLA, Riegl B, Bert C, Hoeksema W, Todd PA (2012) Environmental impacts of dredging and other sediment disturbances on corals: a review. *Mar Pollut Bull* 64:1737-1765.**

A meta-analysis of effects of turbidity, total suspended solids, and sedimentation on corals. They also discussed bottom light requirements. No global recommendations were determined except to say:

> *"Given the wide range of sensitivity levels among coral species and in baseline water quality conditions among reefs, meaningful criteria to limit the extent and turbidity of dredging plumes and their effects on corals will always require site-specific evaluations, taking into account the species assemblage present at the site and the natural variability of local background turbidity and sedimentation."*

8) **FDEP (2011) Site-Specific Information in Support of Establishing Numeric Nutrient Criteria for the Florida Keys. Nutrient Criteria Technical Support Document. 66pp.**

This report outlines two approaches for developing numeric nutrient criteria in Florida Keys waters.

> *"The first consists of adopting the criteria established in the FKRAD, which are based on improving water quality in the inshore halo zone to modeled targets (FDEP 2008a). The second approach is to subdivide the nearshore waters (state waters beyond 500 m) into zones of similar water quality and establish criteria to maintain the current nutrient data distributions, which would continue to support the existing healthy condition."*

FDEP suggested additional requirements for inclusion into rules.

> *"To be applied consistently and to provide an appropriate level of protection, water quality criteria need to include magnitude, frequency, and duration components. The magnitude is a measure of how much of a pollutant may be present in the water without an unacceptable adverse effect. Duration is a measure of how long a pollutant may be above the magnitude, and frequency relates to how often the magnitude may be exceeded without adverse effects."*

9) **FDEP (2013) FDEP Rule, Chapter 62-302, Surface Water Quality Standards.**

The final result of rule-making process for deriving numeric nutrient criteria for South Florida waters. Those for coral reef areas are as follows:

	Florida Keys		
	TP AGM	**TN AGM**	**CHLa AGM**
3. Lower Keys	0.008 mg/L	0.21 mg/L	0.3 µg/L
5. Middle Keys	0.007 mg/L	0.22 mg/L	0.3 µg/L
6. Oceanside	0.007 mg/L	0.17 mg/L	0.3 µg/L
7. Upper Keys	0.007 mg/L	0.18 mg/L	0.2 µg/L

10) **FDEP (2021) DRAFT Technical Support Document for the Revised Turbidity Criterion to Protect Florida Coral and Hardbottom Communities.**

Draft technical report for an ongoing program to revise the turbidity criteria for coral.

> *"The best available science currently in the literature supports a revised turbidity criterion for areas with coral reef habitat at approximately < 7 NTU, based primarily on the work by Fourney and Figueiredo (2017) and Telesnicki and Goldberg (1995). These levels would be more protective of coral recruits, especially for sensitive Acropora sp. However, the value may be reconsidered based on pending study results from NOVA Southeastern University, which currently suggest a criterion of approximately 4.5 NTU for Acropora cervicornis recruits (Robbins 2018)."*

11) **FKRAD (2008) Northern Keys, Central Keys, South Central Keys, and Southern Keys. Reports to FDEP by CDM, Tampa FL.**

Florida Keys Reasonable Assurance Documentation (FKRAD) in lieu of total maximum daily load approach for nutrient management of FKNMS. The FKRAD identified local nutrient sources in the Keys, including wastewater and stormwater. The program used data from FIU water quality monitoring project and included ambient status as well as modeling to propose target concentrations in the local waters (halo zone).

12) **GBRMPA (2009) Water Quality Guidelines for the Great Barrier Reef Marine Park. Great Barrier Reef Marine Park Authority, Townsville. 99 pp.**

"Trigger values" were stratified across distance offshore as: enclosed coastal, open coastal, midshelf, and offshore water bodies.

> *"It is important to emphasize that although improvements in water quality to below the suggested trigger levels will lead to substantial ecosystem benefits, the trigger levels represent an achievable compromise between the current water quality status and that of a pristine system."*

13) **Hawai'i State Department of Health (2021) Hawai'i Administrative Rules, Title 11, Chapter 54: Water Quality Standards.**

Administrative rules determining water quality standards for oceanic reef areas of the state.

> *"It is the objective of class AA waters that these waters remain in their natural pristine state as nearly as possible with an absolute minimum of pollution or alteration of water quality from any human-caused source or actions. To the extent practicable, the wilderness character of these areas shall be protected. No zones of mixing shall be permitted in this class:*
>
> > *(A) Within a defined reef area, in waters of a depth less than ten fathoms (eighteen meters)"*

14) **Hawker DW, Connell DW (1989) An evaluation of the tolerance of corals to nutrients and related water quality characteristics. *Intern J Environ Stud* 34:179-188.**

The authors used ambient offshore conditions to derive criteria related to coral growth reduction.

> *"Since the offshore values are subject to less variability, this has been taken as the background level and is appropriate for off-shore reefs."*
>
> *"Various water quality parameters have previously been shown to correlate with coral growth rate. Using these relationships, water quality factor increases likely to cause 10, 50 and 90% growth reduction for corals of the Great Barrier Reef have been calculated."*

15) **Houk P, Comeros-Raynal M, Lawrence A, Sudek M, Vaeoso M, McGuire K, Regis J (2020) Nutrient benchmarks to protect water quality and coral reefs. *Mar Pollut Bull* 159:111451.**

Based on terrestrial loading estimates from streams on American Samoa.

16) **Houk P, Castro F, McInnis A, Rucinski M, Starsinic C, Concepcion T, Manglona S, Salas E (2022) Nutrient benchmarks to protect water quality, coral reefs, and nearshore fisheries. *Mar Pollut Bull* 184:114144.**

Based on terrestrial loading estimates from streams on Guam.

17) **Japan Basic Environmental Law (2010) Environmental Quality Standards. http://www.env_go_jp/kijun/index_html. Accessed 01/15/2023.**

> *"The basic Environment Law establishes two kinds of Environmental Quality Standard (EQS) relating to water pollution: environmental water quality standards for protecting human health, and environmental water quality standards for protecting the living environment."*

"EQSs have also been established relating to the living environment, including standards for biochemical oxygen demand (BOD), chemical oxygen demand (COD), and dissolved oxygen (DO). Further, EQS have been established for nitrogen and phosphorus levels in lakes/reservoirs and sea/coastal areas, in order to prevent eutrophication."

18) **Koop K, Booth D, Broadbent A, Brodie J, Bucher D, Capone D, Coll J, Dennison W, et al. (2001) ENCORE: the effect of nutrient enrichment on coral reefs. Synthesis of results and conclusions. *Mar Pollut Bull* 42:91–120.**

The ENCORE project was a nutrient fertilization experiment conducted in the lagoon of the relatively pristine One Tree Island Reef, ~70 km offshore the Great Barrier Reef, Australia. The Eutrophication Benchmark Model (ETM) refers to levels of nutrient enrichment where increased algal growth rates cause changes in benthic community structure. Benchmarks were not explicitly stated but ambient concentrations were assumed to be protective.

"Rapid nutrient uptake indicates that nutrient concentrations alone are not adequate to assess nutrient conditions on reefs."

19) **Lapointe BE (1997) Nutrient benchmarks for bottom-up control of macro algal blooms on coral reefs in Jamaica and southeast Florida. *Limnol Oceanogr* 42:1119-1131.**

The author used nutrient bio-enrichment assays as well as historical evidence to develop benchmarks.

"In both locations, concentrations of dissolved inorganic nitrogen (DIN) and soluble reactive phosphorus (SRP) exceeded nutrient benchmarks (~1.0 µM DIN [14 ppb], 0.1 µM SRP [3.0 ppb]) noted to sustain macroalgal blooms on Caribbean coral reefs."

20) **Moss A, Brodie J, Furnas M (2005) Water quality guidelines for the Great Barrier Reef World Heritage Area: a basis for development and preliminary values. *Mar Pollut Bull* 51:76–88.**

Characterized the GBR by geographic region as well as inshore vs offshore zones. Used the 80^{th} percentile approach from ambient data to develop benchmarks.

21) **Nalley EM, Tuttle LJ, Conklin EE, Barkmanc AL, Wulstein DM, Schmidbauer MC, Donahue MJ (2022) A systematic review and meta-analysis of the direct effects of nutrients on corals. *Sci Total Environ* 856:159093. http://dx.doi.org/10.1016/j.scitotenv.2022.159093.**

The authors conducted a meta-analysis of "impact of nutrients" on coral reefs. The 10,911 studies initially identified were winnowed down to 47 which focused on "manipulative experimental studies rather than observational". The criteria were developed through:

"comparable data on coral holobiont responses to nutrients: symbiont density, chlorophyll a

concentration, photosynthesis, photosynthetic efficiency, growth, calcification, adult survival, juvenile survival, and fertilization."

They reported large variability in benchmarks among the 9 physiological responses, in both negative and positive direction of effect.

The authors mentioned the need for "conservative guidelines", but their recommendations of 140 ppb-DIN and 9.3 ppb-PO4- are much higher than those derived from other studies and do not address effects on coral community interactions. With this in mind, we suggest FDEP be aware of these difficulties and keep the bigger picture in mind when developing benchmarks.

22) Tomascik T, Sander F (1985) Effects of eutrophication on reef building corals I. Growth rate of the reef-building coral *Montastrea annularis*. *Mar Biol* 87:143-155.

The authors suggested that moderate nutrient concentrations may positively affect coral growth but that adverse impacts occur beyond benchmark limits.

"A comparison of the 1981-1982 results from the least polluted stations indicates that measurable changes for decreased coral growth rate occur for annual mean suspended particulate matter concentrations (SPM) greater than 4-5 mg/I with a corresponding annual mean chlorophyll a level above 0.4 mg/m3."

23) Tuttle LJ, Donahue MJ (2022) Effects of sediment exposure on corals: a systematic review of experimental studies. *Environ Evid* 11 (4). https://doi.org/10.1186/s13750-022-00256-0.

Peer-reviewed publication of the Tuttle and Donahue (2020) report. A systematic meta-analysis that examined changes in coral health and survival in response to suspended and deposited sediment.

"In response to suspended sediment, adverse effects occurred as low as 10 mg/L for juveniles (reduced growth rates) and 3.2 mg/L for adult corals (bleaching and tissue mortality)."

"Corals take at least 10 times longer to experience tissue mortality from exposure to suspended sediment than to comparable concentrations of deposited sediment, though physiological changes manifest 10 times faster in response to suspended sediment."

24) US-EPA (2016) FY2016 NWPG Measure Definitions South Florida. US-EPA Region 4.

Strategic targets for water quality in the FKNMS developed using 10 years of quarterly sampling events from 150 sites. Specific targets were defined as:

"At least seventy five percent of the monitored stations in the near shore and coastal waters of the Florida Keys National Marine Sanctuary will maintain Chlorophyll a (CHLA) levels at less than or equal to 0.35 ug l^{-1} and light clarity (K_d) levels at less than or equal to 0.20 m^{-1}."

"At least seventy five percent of the monitored stations in the near shore and coastal waters of the Florida Keys National Marine Sanctuary will maintain dissolved inorganic nitrogen (DIN) levels at less than or equal to 0.75 uM [10.5 ppb] and total phosphorus (TP) levels at less than or equal to 0.25 uM. [7.7 ppb]"

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Benjamini Y, Hochberg Y (1995). Controlling the false discovery rate: a practical and powerful approach to multiple testing. *J Royal Stat Soc, Ser B*. 57: 289–300.

Berman T, Bronk DA (2003) Dissolved organic nitrogen: a dynamic participant in aquatic ecosystems. *Aquat Microb Ecol* 31:279–305.

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