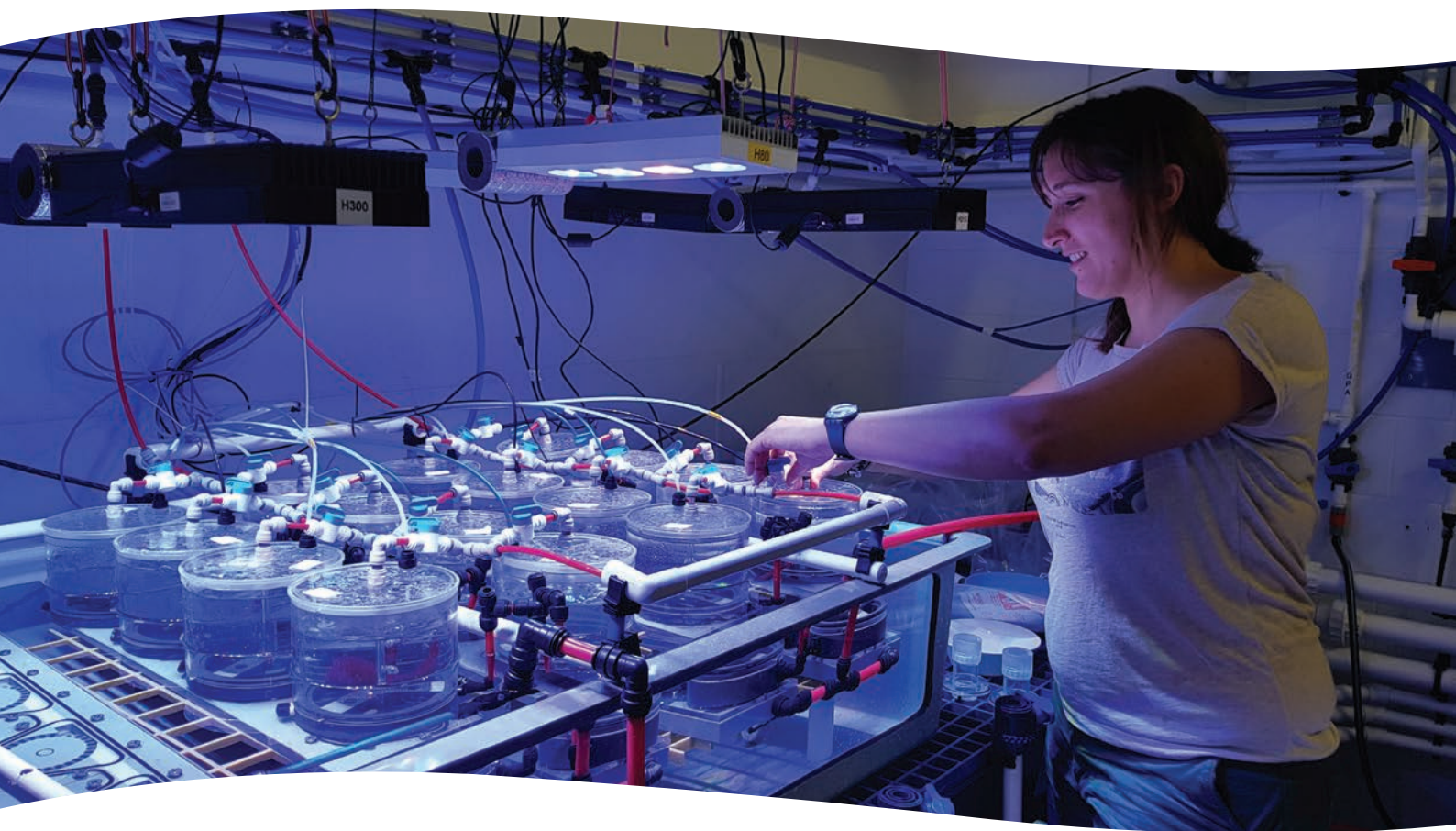


Applying climate adjustments to tropical water quality guidelines

Andrew Negri, Rachael Smith, Olivia King, Julius Frangos, Sven Uthicke



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A multisubstance-potentially affected fraction (ms-PAF) approach

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ACRONYMS

CA	Chemical addition model for calculating joint effects of stressors – assumes same mode of action
CCA	Crustose coralline algae
DoEE	Department of the Environment and Energy
ETX	(where X = 10 or 50) effect temperature that affects X% of a population
ECX	(where X = 10 or 50) effect concentration; concentration that induces a response in x% of a test population
GBR	Great Barrier Reef
HCX	Hazard Concentration: concentration below which X% of species are protected
LC50	Lethal concentration for 50%, e.g. the concentration required to kill half of the subjects in a laboratory test.
LOEC	lowest observed effects concentration
LOET	Lowest observed effect temperature
NESP	National Environmental Science Program
NOEC	No observed effect concentration
NOET	No observed effect temperature
PCX	Protection Concentration: concentration below which X% of species in a community are protected
PTX	Protection Temperature: temperature below which X% of species in a community are protected
PAF	Potentially affected fraction of a community
RA	Response addition model for calculating joint effects of stressors – assumes different modes of action
SSD	Species sensitivity distribution
SST	Sea surface temperature
TWQ	Tropical Water Quality

ABBREVIATIONS

ms-PAF	Multispecies-potentially affected fraction. Also referred to here as multistressor-potentially affected fraction
Ta	The experimental acclimation temperature
Tx	The lowest temperature exceeding Ta (the experimental acclimation temperature) where there is no significant effect on species x (NOEC or ET10).
TTx	The thermal stress threshold = the maximum temperature above experimental acclimation which negative effects first occur following a chronic exposure (TTx = Tx – Ta)

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EXECUTIVE SUMMARY

Climate change and poor water quality represent two of the most common and serious pressures faced by coral reefs globally. While these pressures often co-occur, the potential hazards posed by contaminants and increasing sea surface temperature (SST) to tropical marine species are often considered independently. The joint effects of multiple contaminants can be predicted by the multisubstance-potentially affected fraction (ms-PAF) method, which has been validated for many combinations of contaminants and is currently used to generate a single hazard or risk metric in the monitoring and reporting of pesticides on the Great Barrier Reef. In this project we investigated for the first time the potential application of “multistressor-PAF” (also ms-PAF) to include thermal stress to allow the calculation of tropical climate-adjusted water quality guidelines for two reference toxicants, copper and the herbicide diuron.

National water quality guidelines are derived from species sensitivity distributions (SSDs) where the toxicity thresholds of many species, representing a community, are ranked against concentration, allowing the estimation of concentrations that protect proportions of this community (e.g. the PC95 concentration is protective of 95% of the community). The ms-PAF method of predicting joint effects involves combining information from multiple SSDs, but until now there has been no SSD available for thermal stress on tropical marine species. This project developed the first thermal stress SSD from the thermal stress thresholds of 30 tropical benthic coral reef species across nine phyla. The thermal stress threshold (TTx) was defined as the maximum temperature above experimental acclimation which negative affects first occur following a chronic exposure. This allowed the derivation of protection temperatures: PT99, PT95, PT90 and PT80 of 0.58, 1.2, 1.6 and 2.3°C respectively (e.g. 99% of species should not be affected at temperatures below the PT99 of 0.58°C above normal acclimation temperature). The derived PTx values are similar to temperatures known to initiate coral bleaching and could be considered relevant for broad application in multi-stress risk assessments for tropical reef communities.

The thermal SSD data and existing SSD data for copper and diuron were then combined using the ms-PAF response addition (RA) model to predict the joint response for any combination of thermal stress with chemical concentration. This allowed us to quantify the potential effects of multiple levels of thermal stress on water quality guideline values PC80, PC90, PC95 and PC99 for these contaminants. The influence of thermal stress on the copper and diuron SSDs was to shift the SSD for each increment above acclimation temperatures. The shifts in contaminant SSDs were minor for small temperature increments (TTx < +1.0°C), but the shifts became more pronounced with increasing temperatures above acclimation. The influence of thermal stress on water quality guidelines changed depending on the stressor combination. Some examples include: at a temperature increase of 0.5°C above acclimation the PC99 for copper would need to be reduced by 67% to protect 99% of species; the same temperature increase would necessitate an adjustment of the PC99 for diuron by 23% to protect 99% of species.

The extension of ms-PAF methods to include non-chemical stressors such as high SST enabled the adjustment of current guidelines for copper and diuron to account for thermal stress events. However, this preliminary thermal SSD for tropical species should be considered a proof-of-concept step. The SSD should be further developed by the inclusion of

additional existing data (experimental and field), and by modifying future experimental designs to include acclimation temperatures closer to summer maxima and smaller increments in temperature for more meaningful and precise calculation of thermal stress thresholds. Nevertheless, the thermal stress SSD generated plausible community protection values that can be considered for application in multi-stress risk assessments. This approach could be extended further to other non-contaminant stressors such as sediment exposure, low salinity, light limitation, anoxia and ocean acidification to advance more comprehensive environmental guidelines, reporting and assessments.

1.0 INTRODUCTION

The health of coastal marine ecosystems is declining globally due to multiple, often simultaneous, anthropogenic pressures (Halpern et al., 2015). Tropical marine ecosystems are for example under pressure from ocean warming and acidification, and these global stressors can occur simultaneously with declining water quality to further pressure coral reefs (Ban et al., 2014; Hughes et al., 2017a). Consequently, improving water quality is considered one of few actions that can be undertaken locally to help mitigate, in the short term, decline of coastal ecosystems from climate change (Hughes et al., 2017a; MacNeil et al., 2019). Maintaining contaminant concentrations below local water quality guidelines is one of several target objectives of water quality management programs, intended to improve the resilience of reefs to thermal bleaching (Brodie et al., 2017). However, current water quality guidelines are derived from single-stressor ecotoxicological experiments performed under benign conditions and do not account for other simultaneous stressors which can affect the toxicity of contaminants (Heugens et al., 2001; Kwok et al., 2007; Lau et al., 2014; Zhou et al., 2014). Applying safety factors (lowering the values of water quality guidelines) has been proposed to ensure they remain protective of sensitive species facing multiple pressures, but these can often be arbitrary or unreasonably severe (Heugens et al., 2001).

The most widely studied stressor that commonly co-occurs with contaminants in the marine environments is temperature (Ban et al., 2014; Heugens et al., 2001). Temperatures in tropical coral reef waters have already increased by nearly 1°C since the industrial revolution (Lough et al., 2018), and further 2-3°C increases are predicted by 2100 (Collins et al., 2013; Magnan et al., 2016); thus it becomes crucial to consider adjustments to water quality guideline values for current heatwave conditions and future temperature increases (“climate-adjusted-thresholds”). The sensitivity of marine ectotherms to contaminants can change at temperatures approaching their lower and upper thermal tolerance ranges (Cairns et al., 1975; Heugens et al., 2001). This is due to the influence of temperature on uptake and elimination as well as changes in biochemistry, physiology and ecology and to the speciation and bioavailability of the contaminant (Cairns et al., 1975; Heugens et al., 2001). More recently Zhou et al. (2014) advanced several conceptual models for predicting the temperature dependent toxicity of contaminants. Their meta-analysis demonstrated that toxicity of metals to aquatic species most often increased below and above the thermal optima or increased linearly with increasing temperature.

There are a substantial number of single-species studies that have tested the influence of temperature on toxicity (Noyes et al., 2009); however, understanding the effects of thermal stress on water quality guidelines requires data representative of marine communities. Guidelines are usually based on the sensitivity of marine communities using species sensitivity distributions (SSD) (Posthuma et al., 2002); cumulative statistical models that describe the relationship between the potentially affected fraction (PAF) of multiple species across multiple taxa relative to contaminant concentration. This enables the derivation of water quality guidelines based on the proportion of species in that community that are likely to be affected (Warne et al., 2018a). For example, maintaining contaminant concentrations below the 95% protection concentration (PC95) should protect 95% of species in that community (ecosystem or habitat) (note PC95 = 5% hazard concentration, HC5). However, the data used to construct SSDs are typically chosen from experiments conducted under conditions close to their thermal

optimum. Comparisons of SSDs have been developed at different temperatures (tested within the normal thermal window of each species) and show differences in sensitivity to a range of contaminants between temperate and tropical communities (Kwok et al., 2007; Raymundo et al., 2019) and cold water and temperate marine species (Bejarano et al., 2017). Zhou et al. (2014) modelled the influence of temperature on toxicity for three metals to describe how temperature-shifted SSDs, hence water quality protection concentrations, changed over 10 and 15°C temperature ranges. For example, the protection concentration for 90% of species (PC90, HC10) reduced almost 10-fold for cadmium with increasing temperatures, and the authors suggested that applying a 10-fold safety factor could be an appropriate response to ensure contaminant guidelines are protective of communities across wide temperature ranges.

Deriving SSDs for contaminants at multiple temperatures is presently limited by inadequate experimental toxicity data for most species and chemicals across temperatures (Zhou et al., 2014). An alternative approach to estimate the combined impacts of thermal stress and contaminants on marine communities might be to combine individual chemical SSDs and thermal SSDs using the multispecies potentially affected fraction (ms-PAF) method (Traas et al., 2002), which is currently used to predict the combined effects of chemical mixtures (joint action response) from individual SSDs by applying well-established models. The model chosen depends on whether the mode of action (MoA) of the toxicants are the same or different, and the stressors should not interact toxicologically (de Zwart and Posthuma, 2005; Plackett and Hewlett, 1952). The concentration addition (CA) model of joint action is usually applied in the case where the MoA is the same, for example a mixture of herbicides that all bind to the QB binding site of the D1 protein in photosystem II (PSII) (Wilkinson et al., 2015). Conversely, the response addition (RA) model of joint action is often applied for mixtures of chemicals with independent modes of action (de Zwart and Posthuma, 2005), a herbicide and insecticide for example. While CA and RA models for joint action were originally intended to address mixture toxicity for single species, their application to predict the ecological risk of complex mixtures by applying these to multiple species SSDs has been proposed (Traas et al., 2002), critically reviewed (Backhaus and Faust, 2012), and applied to mixtures of contaminants with up to 10 different modes of action (Parkerton et al., 2018).

Although most of the studies on joint action have tested chemical mixtures, there is the potential for these approaches to be applied to combinations of other pressures such as contaminants and thermal stress, and this has been successfully employed for individual marine species (Uthicke et al., 2016; van Dam et al., 2012; van Dam et al., 2015). To extend this application from individual species to marine communities, SSDs are needed that relate PAF of a marine assemblage to thermal stress (there are already many marine SSDs for individual contaminants (Posthuma et al., 2019)). Thermal stress SSDs for elevated temperatures have been described for freshwater fish (Leuven et al., 2011) and molluscs (Verbrugge et al., 2012), as well as mostly temperate coastal species across a 15°C range (de Vries et al., 2008). So far no thermal stress SSDs have been constructed for sub-tidal tropical marine species, which are generally exposed to a far narrower annual temperature ranges of less than 8°C (decreasing with latitude) (AIMS, 2019). Consequently, thermal thresholds above species optima are likely to be lower for many tropical species (Gaston, 2009), leading to distinctive thermal SSDs between tropical and temperate communities.

In this case study, we explored the possibility of applying ms-PAF to derive the influence of thermal stress on water quality guidelines for contaminants. Firstly, we adapted the selection

criteria and quality assessment approach, traditionally used for selecting ecotoxicity data for developing default water quality guidelines (Hobbs et al., 2005; Warne et al., 2018a), to select thermal stress data for individual tropical marine species characteristic of benthic reef communities. We then searched the literature and collated the relevant published experimental data on thermal stress thresholds (defined here as the maximum temperature above experimental acclimation which negative effects occur) for tropical marine species. A cumulative probability function was fitted to the multi-species data set to derive an SSD for thermal stress. Temperature risk values ($^{\circ}\text{C}$ above acclimation): PT80, PT90, PT95 and PT99 were interpolated from the SSD, indicating protection of 80, 90, 95 and 99% of species respectively in a tropical marine community. The thermal SSD data and existing SSD data for the metal, copper, and the herbicide, diuron were then combined using the ms-PAF RA model to predict the joint response for any combination of thermal stress with chemical concentration. This allowed us to quantify the potential effects of multiple levels of thermal stress on water quality guideline values PC80, PC90, PC95 and PC99 for these contaminants. The rationale and validity of this approach was assessed and recommendations to improve the thermal stress SSD and its application for assessing multi-stressor impacts were considered.

2.0 METHODOLOGY

2.1 General approach

An SSD for thermal stress to tropical marine species was developed to identify the percentage of species in a tropical community (PAF) negatively affected by increasing temperatures. The thermal SSD was then used alongside established SSDs for copper and diuron using the ms-PAF technique to predict how thermal stress could influence the water quality guidelines for these contaminants.

2.2 SSD for thermal stress

The development of an SSD for thermal stress to marine communities requires thermal stress data for multiple species across diverse phyla (de Vries et al., 2008). A literature search was conducted to identify studies that had quantified the effects of elevated temperatures on benthic marine species associated with tropical coral reefs. The Web of Science and Google Scholar were searched (after 1980 using terms including temperature, thermal, heat, stress, tropical, sub-tropical, coral, reef, marine, coastal) and this search was supplemented, with papers cited in recent reviews (Ban et al., 2014; Uthicke et al., 2016). Only studies with species that occur in the tropics and occur on coral reefs were included in the dataset, and only tests performed at 18°C or higher, which has been identified as the minimum temperature for coral reef growth (Kleypas et al., 1999), were considered appropriate for inclusion.

For consistency with established copper and diuron SSDs (below), the assessment for suitable thermal stress data was based on a modification of the recently revised method for derivation of the Australian and New Zealand Water Quality Guidelines (Hobbs et al., 2005; Warne et al., 2018a). Key criteria for selection included adequate descriptions of: (i) the temperature and duration of both acclimation and exposure, (ii) replication and (iii) the statistical method or model used to determine effect. Studies were only included if they: (i) reported ecologically-relevant endpoints (mortality, growth, reproduction) and (ii) were conducted over “chronic” exposure durations (as defined in Warne et al., 2018a) to avoid the conversions of thresholds from acute to chronic. The data quality assessment process was formalised by answering 18 questions on how the data were generated (e.g. test organism, experimental, design, chemical and statistical analysis) based on the information provided in the articles (Hobbs et al., 2005; Warne et al., 2018a), and an example template can be found in the Appendix (Table A1). Only “acceptable” quality data (score $\geq 50\%$) were included in the SSD, and only experimental studies were used to ensure reliable and consistent thermal exposures; however, ways of including field data should be explored in the future. Most of the publications reported multiple endpoints for multiple species; however, the dataset was reduced to obtain a single threshold value to represent the sensitivity of each species in the SSD (Warne et al., 2018a). Similar to the methods of deriving water quality guidelines (ANZECC and ARMCANZ 2000), obtaining a single threshold value for each species is conducted via some selection and manipulation of the threshold data based on each combination of species, endpoint and duration (Warne et al., 2018). For example, species where there are multiple values for the same endpoint and test duration, the geometric mean of the values is calculated and adopted. If there are multiple durations and endpoints for a species, the lowest value is adopted to represent the sensitivity of the species in the SSD.

Metrics for thermal stress have previously included the temperature at which 50% of organisms are killed (ET50) or the time taken to reach 50% mortality (de Vries et al., 2008; Urban, 1994). The thermal tolerance interval (TTI) developed by Urban (1994) defined the temperature interval by which the temperature can increase above the acclimated temperature without killing more than 50% of the population. Calculating the joint effect of multiple stressors using ms-PAF requires the SSDs be derived for consistent effect metrics (Traas et al., 2002), and the current water quality guidelines used SSDs based on a combination of chronic no effect concentrations, 10% effect concentrations (EC10) and no observed effect concentrations (NOEC) (Hobbs et al., 2005; Warne et al., 2018a). Therefore, for consistency with existing contaminant SSDs, the data used to create the thermal stress SSD in the present study included the temperatures that caused a 10% ecologically relevant effect (ET10) or no observed effect (NOET) for each species in individual tests. We defined the temperature threshold (TTx) for each species as the maximum temperature above acclimation which negative affects occur according to Equation 1:

$$TTx = Tx - Ta \quad \text{Eq 1.}$$

Where Tx (°C) is the lowest temperature exceeding Ta (the experimental acclimation temperature) where there is no significant effect on species x (NOEC or ET10). If the NOET was equivalent to the acclimation temperature (Ta), the data were excluded, as this provided no information to identify a thermal effect threshold above acclimation. Data on other modelled thresholds, such as the temperature that caused a 50% effect on a species (ET50) were collected but not used in derivation of the thermal stress SSD.

As is the case for contaminant toxicity, the thermal threshold is also dependent on the exposure period, i.e. the longer the exposure period, the greater the effect on organisms for a defined increase in temperature (Urban, 1994). A chronic exposure period (which can be different for different taxa and life history stages) is used in the derivation of the Australian and New Zealand water quality guidelines for contaminants and have been used to populate the copper and diuron SSDs (Warne et al., 2018a). Using chronic, rather than acute, thermal stress data in the thermal SSD is therefore required for applying ms-PAF to derive the joint action of temperature with copper and diuron. The resulting thermal stress SSD is relevant to extended periods of increased sea surface temperature (e.g. because of climate change or summer heatwave conditions), and not the short-term effects of, for example, pulsed releases of heated water from industry.

For consistency with the copper and diuron SSDs (below), thermal stress SSDs were derived using the BurrIoz 2.0 software (CSIRO, 2019). This software applied the Burr type III statistical distribution (Eq. 2) that best fit the effect TTx data of multiple species, where PAF (%) is the potentially affected fraction of the community (%), b , c and k are location and shape parameters.

$$PAF (\%)_{Burr III} = \frac{100}{\left[1 + \left(\frac{b}{TTx}\right)^c\right]^k} \quad \text{Eq. 2}$$

BurrIoz 2.0 calculated the temperatures for four levels of ecosystem protection, i.e. the protective temperature (PTx) for 80%, 90%, 95% and 99% of species in an ecosystem (PT80, PT90, PT95 and PT99 respectively). To protect high conservation value systems and

moderately disturbed value systems, PT99 and PT95 values are recommended, respectively (Warne et al., 2018a).

2.3 SSD for copper and diuron

The effect concentration data to generate the SSD for copper (25 marine species from 8 phyla) was obtained from the Australian and New Zealand Water Quality Guidelines (ANZ, 2018). The effect concentration data to derive the SSD for diuron (20 marine species that belonged to six phyla) was obtained from recently proposed water quality guidelines (Warne et al., 2018b). The SSDs for these contaminants were also derived using Burr type III distributions (BurrIioz 2.0, (CSIRO, 2019)).

2.4 ms-PAF to predict the joint effects of thermal stress and contaminants using the Response Addition RA model

The response addition (RA) joint action model is used for pressures that have different modes of action and that do not interact at the target site of toxic action (de Zwart and Posthuma, 2005; Traas et al., 2002). Also known as the Independent Action (IA) model, the RA model was used here to derive expected joint action response between thermal stress and the two contaminants as the modes of action of all three stressors are likely to differ, and was previously shown to be a good predictive model for single species responses to these stressor combinations (Uthicke et al., 2016; van Dam et al., 2012; van Dam et al., 2015). Using the RA model of joint action, the “multiple stressor” potentially affected fraction of a community (*ms-PAF_{RA}*) was calculated by combining the PAF of each stressor according to Equations 3 (Traas et al., 2002):

$$MS-PAF_{RA} = PAF_A + PAF_B - (PAF_A \times PAF_B) \quad \text{Eq. 3}$$

Where *PAF_A* and *PAF_B* are the potentially affected fractions from two stressors with different modes of action (e.g. thermal, copper and/or diuron), scaled from 0 (0% of the community affected) to 1 (100% of the community affected). Scaling *PAF* between 0 and 1 in this equation results in an asymptotic model that cannot exceed an effect on more than 100% according as required by the joint probability of statistically independent events (Backhaus and Faust, 2012). This approach can also be used to calculate *ms-PAF_{RA}* for more than two stressors with different modes of action Equation 4:

$$PAF_{RA} = 1 - \sum_i (1 - PAF_i) \quad \text{Eq. 4}$$

Where *PAF_i* is the *PAF* of *i* stressors from 1 to *n* (Traas et al., 2002).

3.0 RESULTS

3.1 Data contributing to the thermal SSD

The literature search for appropriate experimental thermal threshold data for tropical marine species yielded 144 publications. Each publication was first screened to eliminate any data sources that did not meet essential criteria: i.e. did not use ecologically relevant endpoints (e.g. survival, growth, reproduction); provided inadequate descriptions of the thermal acclimation or treatments; or did not derive biological effect/thresholds from dose-response curve fitting or statistics (e.g. ET10 or NOET). Following this, data were quality assessed, resulting in thermal stress data for 30 species, representing 9 phyla (**Table 1**), which meets the minimum data requirements to derive a SSD according to established criteria for deriving water quality guidelines (Warne et al., 2018a). The species included tropical habitat building corals, crustose coralline algae (CCA), calcifying green algae (*Halimeda* sp.) and seagrass, reef-associated invertebrates including foraminifera and sea urchins, benthic diatoms and coral symbionts (**Table 1**).

3.2 Thermal SSD and guideline values for thermal stress and contaminants

The acclimation temperatures (T_a) ranged from 23-29°C across the species tested (Table 1, Figure 1), which corresponds to the temperature range of coral reefs such as the Great Barrier Reef (AIMS, 2019). The TTx ET10/NOET values in the thermal stress dataset ranged from 1 – 7.9°C with corals and sponges being among the most sensitive taxa (Table 1). Although some coral species had TTx values as low as 1 – 2°C above acclimation temperatures, the survival of other coral species were only affected at +5.9°C. There was no correlation between the acclimation temperature T_a and the thermal threshold in this dataset (Figure 1). The Burr III distribution was well correlated with the data (Figure 2. Table A2), which combined with the amount and type of ecotoxicity data available (Table 1) resulted in a set of ‘very high’ reliability protection temperature (PTx) values (Table 2). Interpreting these values as guidelines for risk of thermal stress, a PT_{99} of 0.58°C indicates 99% of the tropical marine community would be at risk of from chronic exposures above this temperature, while a PT_{95} of 1.2°C is indicative of 95% species protection and so on.

The diuron and copper SSDs (Figure A1, Table A2), also from the Burr III function, enabled the derivation of very high reliability protection concentration values (PCx , Table 2). The PCx values for diuron were identical to those previously published in Warne et al. (2018b), while the PCx values for copper were very similar to those in the Australia and New Zealand national water quality guidelines (0.3, 1.3, 3, 8 $\mu\text{g L}^{-1}$ for Cu PC_{99} , PC_{95} , PC_{90} , PC_{80} respectively (ANZ, 2018)). These minor differences in PCx values are likely due to updates in the Burr III software since the copper guidelines were originally derived in 2000.

Table 1: Summary of the thermal threshold values TT_x for each species used to derive the thermal SSD (Figure 2). T_a = acclimation temperature. CCA = crustose coralline algae.

Species	Phylum	Taxa	Life stage	Endpoint	T_a	TT_x	Source
<i>Acropora intermedia</i>	Cnidaria	Coral	Adult	Bleaching	25.5	3	(Anthony et al., 2008)
<i>Acropora millepora</i>	Cnidaria	Coral	Adult	Survival	25.3	5.9	(Fabricius et al., 2013)
<i>Acropora spathulata</i>	Cnidaria	Coral	Early life stage	Embryo development	28	4	(Woolsey et al., 2015)
<i>Acropora tenuis</i>	Cnidaria	Coral	Gametes	Fertilisation	27	5.3	(Negri et al., 2011b)
<i>Cyphastrea microphthalma</i>	Cnidaria	Coral	Early life stage	Embryo development	28	2	(Woolsey et al., 2015)
<i>Fungia fungites</i>	Cnidaria	Coral	Larvae	Survival	28.1	6	(Baria et al., 2015)
<i>Goniastrea australensis</i>	Cnidaria	Coral	Early life stage	Embryo development	28	2	(Woolsey et al., 2015)
<i>Goniastrea favulus</i>	Cnidaria	Coral	Early life stage	Embryo development	28	4	(Woolsey et al., 2015)
<i>Lithophyllon repanda</i>	Cnidaria	Coral	Larvae	Survival	28.1	2.9	(Baria et al., 2015)
<i>Montipora tuberculosa</i>	Cnidaria	Coral	Adult	Survival	25.3	5.9	(Fabricius et al., 2013)
<i>Porites panamensis</i>	Cnidaria	Coral	Juvenile	Survival	28.9	1	(Anlauf et al., 2011)
<i>Fungia fragum</i>	Cnidaria	Coral	Larvae	Survival	27.8	3.28	(Randall and Szmant, 2009)
<i>Amphistegina lobifera</i>	Foraminifera	Foram	Adult	Bleaching	24	2	(Prazeres et al., 2016)
<i>Calcarina hispida</i>	Foraminifera	Foram	Adult	Bleaching	26	5	(Schmidt et al., 2011)
<i>Amphistegina radiata</i>	Foraminifera	Foram	Adult	Bleaching	26	3	(Schmidt et al., 2011)
<i>Marginopora vertebralis</i>	Foraminifera	Foram	Adult	Mortality	26	5	(Uthicke et al., 2012)
<i>Halimeda cylindracea</i>	Chlorophyta	Green alga	Adult	Calcification rate	28	4	(Sinutok et al., 2011)
<i>Halimeda macroloba</i>	Chlorophyta	Green alga	Adult	Calcification rate	28	4	(Sinutok et al., 2011)
<i>Porolithon onkodes</i>	Rhodophyta	CCA	Adult	Bleaching	25.5	3	(Anthony et al., 2008)
<i>Zostera muelleri</i>	Tracheophyta	Seagrass	Adult	Growth	27	3	(Collier et al., 2011)
<i>Halodule uninervis</i>	Tracheophyta	Seagrass	Adult	Growth	27	6	(Collier et al., 2011)
<i>Carteriospongia foliascens</i>	Porifera	Sponge	Adult	Tissue necrosis	28.6	1.39	(Bennett et al., 2017)
<i>Stylissa flabelliformis</i>	Porifera	Sponge	Adult	Tissue necrosis	28.6	1.39	(Bennett et al., 2017)
<i>Rhopaloeides odorabile</i>	Porifera	Sponge	Adult	Tissue necrosis	28.6	2.88	(Bennett et al., 2017)
<i>Cymbastela coralliophila</i>	Porifera	Sponge	Adult	Growth	28.6	1.39	(Bennett et al., 2017)
<i>Cliona orientalis</i>	Porifera	Sponge	Adult	Growth	23	7.9	(Ramsby et al., 2018)
<i>Lytechinus variegatus</i>	Echinodermata	Urchin	Gametes	Fertilisation	29	3.6	(Collin and Chan, 2016)
<i>Brevium minutum</i>	Dinoflagellata	Dinoflagellate	Vegetative	Growth	27	3	(Grégoire et al., 2017)
<i>Durusdinium trenchii</i>	Dinoflagellata	Dinoflagellate	Vegetative	Growth	27	3	(Grégoire et al., 2017)
<i>Nitzschia closterium</i>	Heterokonta	Diatom	Vegetative	Growth	27	5.7	(Harford et al., 2011)

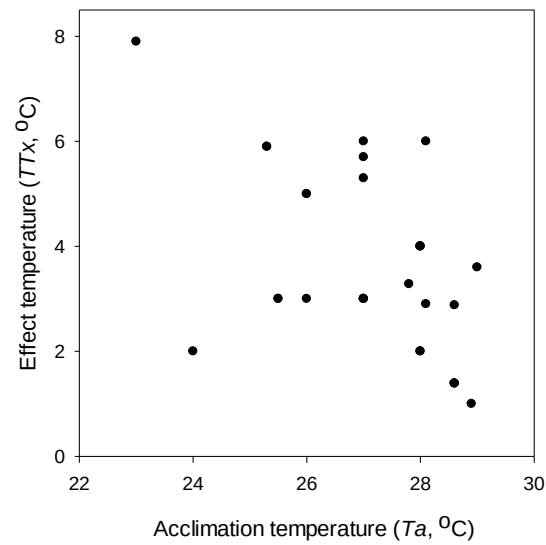


Figure 1: Acclimation temperature T_a vs temperature threshold TT_x .

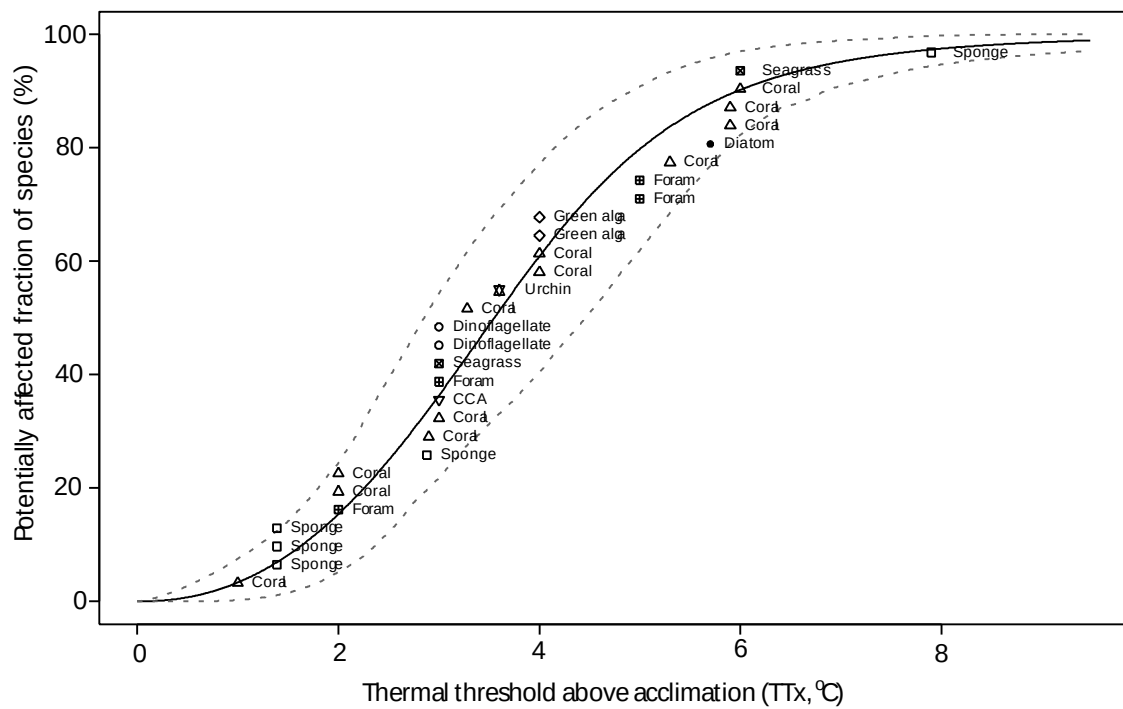


Figure 2: Species sensitivity distribution (SSD) plot of the thermal stress threshold data ($TT_x = T_x - T_a$) used to derive tropical marine thermal stress temperature effect values (PT_x). Dashed line = 95% CI.

3.3 Predicting the influence of thermal stress on diuron and copper guideline values using ms-PAF

The influence of thermal stress on the copper SSD, predicted by the RA joint effect model (Traas et al., 2002) was to shift the SSD vertically for each increment above the acclimation temperature (Figure 3). The shift in SSD was minor for small temperature increments ($TTx < +1.0^{\circ}\text{C}$), but the shifts became more pronounced with increasing temperatures above acclimation. The SSDs converged at high copper concentrations ($> 10 \mu\text{g L}^{-1}$) as the metal starts to have a greater influence on the percentage of affected species at the temperatures plotted (up to $TTx = +2.5^{\circ}\text{C}$).

Table 2: Protection concentrations PCx (CI range) for copper and diuron exposures (SSDs in Figure A1) and Protection temperatures PTx for elevated temperature exposure (SSD Figure 2). The table also includes the influence of elevated temperature on PCx ($\mu\text{g L}^{-1}$) for copper and diuron exposures and the effect of diuron and copper on PTx ($^{\circ}\text{C}$) for elevated temperature exposures based on ms-PAF calculations. Grey percentages in brackets indicate the % adjustment in guideline value.

Copper ($\mu\text{g L}^{-1}$)	PC99	PC95	PC90	PC80	PC50
Acclimation temp.	0.29 (0.024-2.2)	1.4 (0.44-5.4)	3.0 (1.2-9.4)	7.4 (3.0-20)	42 (20-108)
$TTa + 0.5^{\circ}\text{C}$	0.095 (67%)	1.2 (14%)	2.8 (7%)	7.1 (4%)	42 (0%)
$TTa + 1.0^{\circ}\text{C}$	-	0.58 (59%)	2.1 (30%)	6.0 (19%)	39 (7%)
$TTa + 1.5^{\circ}\text{C}$	-	-	0.55 (82%)	4.1 (45%)	33 (21%)
$TTa + 2.0^{\circ}\text{C}$	-	-	-	1.7 (77%)	26 (38%)
$TTa + 2.5^{\circ}\text{C}$	-	-	-	-	17 (60%)
Diuron ($\mu\text{g L}^{-1}$)	PC99	PC95	PC90	PC80	PC50
Acclimation temp.	0.43 (0.079-0.77)	0.67 (0.39-1.1)	0.86 (0.70-1.4)	1.20 (0.99-2.1)	2.4 (1.8-2.4)
$TTa + 0.5^{\circ}\text{C}$	0.33 (23%)	0.64 (4%)	0.84 (2%)	1.16 (3%)	2.36 (2%)
$TTa + 1.0^{\circ}\text{C}$	-	0.52 (22%)	0.76 (12%)	1.11 (7%)	2.30 (4%)
$TTa + 1.5^{\circ}\text{C}$	-	-	0.51 (41%)	0.96 (20%)	2.15 (10%)
$TTa + 2.0^{\circ}\text{C}$	-	-	-	0.71 (41%)	1.94 (19%)
$TTa + 2.5^{\circ}\text{C}$	-	-	-	-	0.61 (75%)
Thermal stress ($^{\circ}\text{C}$)	PT99	PT95	PT90	PT80	PT50
Uncontaminated	0.58 (0.24-1.4)	1.2 (0.75-2.0)	1.6 (1.2-2.3)	2.3 (1.7-2.9)	3.6 (2.9-4.4)
+0.29 $\mu\text{g L}^{-1}$ Cu	-	1.09 (9%)	1.57 (2%)	2.22 (3%)	3.53 (2%)
+1.4 $\mu\text{g L}^{-1}$ Cu	-	-	1.23 (23%)	2.02 (12%)	3.45 (4%)
+3.0 $\mu\text{g L}^{-1}$ Cu	-	-	-	1.72 (25%)	3.33 (8%)
+7.4 $\mu\text{g L}^{-1}$ Cu	-	-	-	-	3.05 (15%)
+0.43 $\mu\text{g L}^{-1}$ diuron	-	1.09 (9%)	1.57 (2%)	2.22 (3%)	3.53 (2%)
+0.67 $\mu\text{g L}^{-1}$ diuron	-	-	1.23 (23%)	2.02 (12%)	3.45 (4%)
+0.86 $\mu\text{g L}^{-1}$ diuron	-	-	-	1.72 (25%)	3.33 (8%)
+1.20 $\mu\text{g L}^{-1}$ diuron	-	-	-	-	3.05 (15%)

At a temperature of 0.5°C above acclimation the PC99 for copper would need to be adjusted to $0.095 \mu\text{g L}^{-1}$ (a reduction of 67%, Table 2Error! Reference source not found.) to protect 99% of species. At a temperature of 1.0°C above acclimation, more than 1% of the community is expected to be affected in the absence of copper ($PT99 = 0.58^{\circ}\text{C}$, Figure 2), and consequently there is no predicted effect on the copper PC99 at this temperate (Table 2). At $TTi = +1.0^{\circ}\text{C}$ the PC95 for copper would be adjusted from 1.4 to $0.58 \mu\text{g L}^{-1}$ to protect 95% of species from the joint effects of both stressors. Other temperature stress adjustments for PC90, PC80 and PC50 can be found in Table 2.

The influence of thermal stress was also predicted to shift the diuron SSD vertically for each increment above the acclimation temperature (Figure 3). Again, the shifts became more pronounced with increasing temperatures, and the SSDs converged at high diuron concentrations ($> 2 \mu\text{g L}^{-1}$). At a temperature of 0.5°C above acclimation the PC99 for diuron

would need to be adjusted to $0.33 \mu\text{g L}^{-1}$ (a reduction of 23%, Table 2) to protect 99% of species. While at $TTi = +1.0^\circ\text{C}$ the PC95 for diuron would need to be reduced from 0.67 to $0.64 \mu\text{g L}^{-1}$. The greatest predicted influence of temperature on diuron guidelines occurs as the PCx increases and at higher temperatures, for example the PC80 for diuron would need to be reduced from 1.20 to $0.71 \mu\text{g L}^{-1}$ at 2°C above acclimation to protect 80% of species from this combination of herbicide and thermal stress (Table 2).

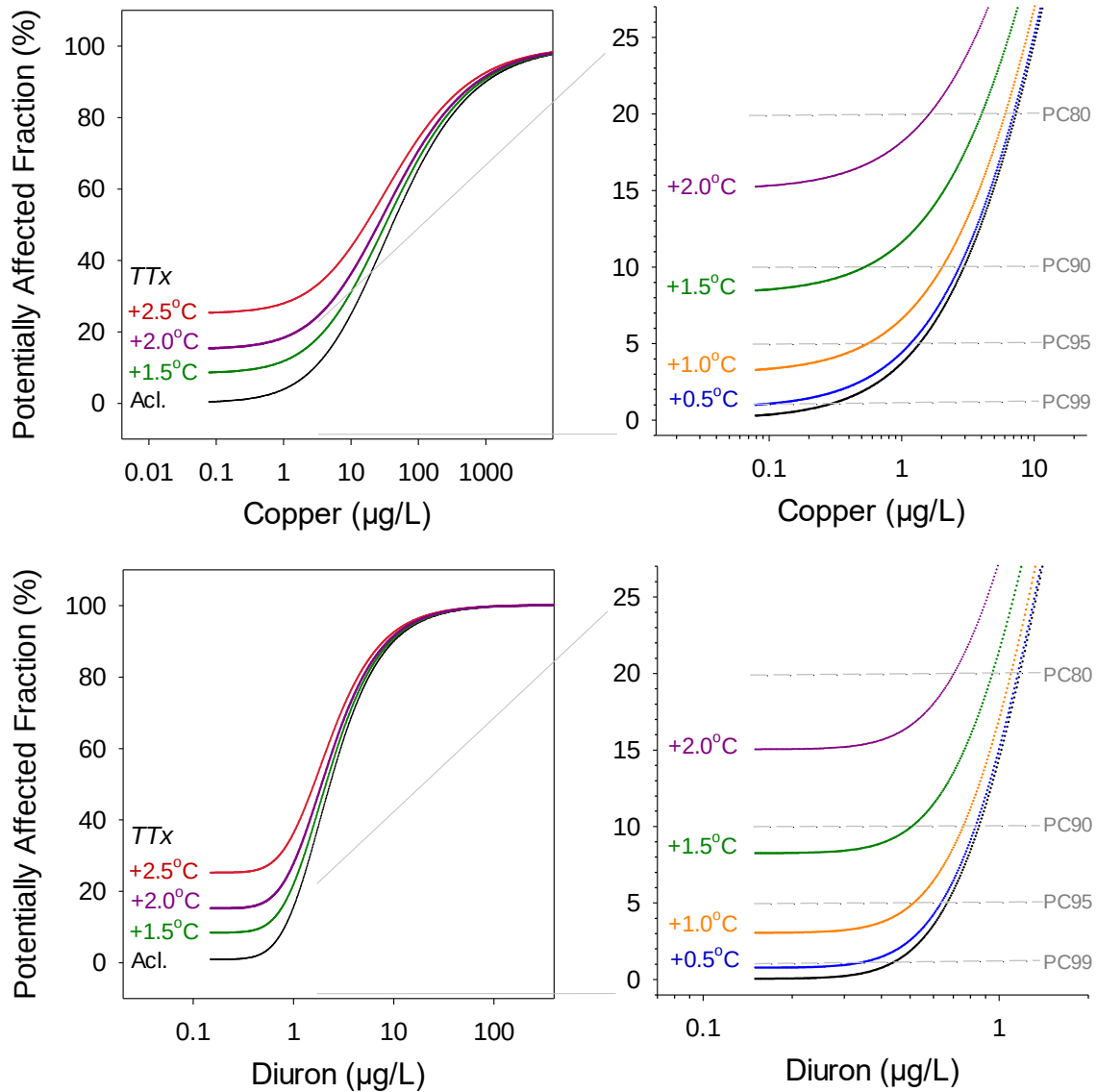


Figure 3: SSDs for copper and diuron at acclimation temperature (Acl.) and shifts in these SSDs at elevated temperatures (TTx) predicted from ms-PAF. Left = full scale, Right = expanded view of grey areas.

At a temperature of 1.0°C above acclimation, more than 1% of the community is expected to be affected in the absence of diuron ($PT99 = 0.58^\circ\text{C}$, Figure 2), and consequently there is no predicted effect on the PC99 for diuron. However, at $TTi = +1.0^\circ\text{C}$ the PC95 for diuron would be expected to reduce from 0.67 to $0.63 \mu\text{g L}^{-1}$ and cause similar reductions for PC90, PC80 and PC50 (Table 2). The greatest predicted influence of temperature on diuron guidelines occurs as the PCx increases and at higher temperatures, for example the PC80 for diuron was reduced from 1.20 to $0.71 \mu\text{g L}^{-1}$ at 2°C above acclimation ($TTx = +2.0^\circ\text{C}$, Table 2).

3.4 Predicting the influence of diuron and copper on the thermal stress protection temperature values using ms-PAF

The influence of diuron on the thermal stress SSD, predicted by the RA joint effect model mirrored the effects of thermal stress on diuron PAF (above) (Figure A2). In this case low concentrations of copper and diuron, such as the PC99 values of 0.29 and 0.43 $\mu\text{g L}^{-1}$ respectively, both caused minor shifts in the thermal SSD (Figure A2), and only a small predicted effect on PTx values. For example, PT95 would be expected to reduce from 1.20 to 1.09°C at 0.29 and 0.43 $\mu\text{g L}^{-1}$ of copper and diuron respectively (Table 2). The influence of these contaminants on the thermal stress risk thresholds increases at higher concentrations. For example, PT80 for thermal stress was reduced from 2.3 to 1.7°C at the PT80 concentration of 7.4 and 1.2 $\mu\text{g L}^{-1}$ of copper and diuron respectively (Table 2).

4.0 DISCUSSION

The main aim of our report was to investigate multisubstance-potentially affected fraction (ms-PAF) as an approach to derive climate-adjusted water quality thresholds for tropical coral reefs, and potentially other ecosystems. The development of the first species sensitivity distribution (SSD) for thermal stress for 30 tropical benthic marine species, using methods adapted from water quality guideline derivation, enabled quantitative predictions of community effects as temperatures exceeded acclimation values. These resulting protection temperature values (PT_x) were similar to temperatures known to initiate coral bleaching and are therefore relevant for application in multi-stress risk assessments. The extension of ms-PAF methods to include non-chemical stressors such as high SST enabled the adjustment of current guidelines for copper and diuron to account for thermal stress events. Further refinement of this approach, including validation of joint action model choice and responses, could allow ms-PAF to be applied to spatially quantify pollution reduction targets, with the aims of reducing impacts of the heating events and assisting recovery. This could be extended further to other non-contaminant stressors such as sediment exposure, low salinity, light limitation, anoxia and ocean acidification advance more comprehensive environmental guidelines, reporting and assessments.

4.1 Temperature stress data

To ensure compatibility with water quality guidelines, the assessment of experimental thermal stress data to develop a thermal stress SSD followed a similar standard approach. There were numerous thermal stress datasets for tropical species; however, most studies were not designed to identify NOET or ET10 thresholds for thermal stress. A common issue was that datasets included only one elevated temperature treatment and often the temperature increments between treatments were large, making the identification of precise thresholds difficult. Most data were also from acute exposure durations that were not suitable for deriving a chronic SSD. However, using this approach we identified thresholds for 30 tropical species across 9 phyla to represent the sensitivity to thermal stress of a tropical benthic reef community, a diversity considered to be appropriate for deriving water quality guidelines (Warne et al., 2018a). It was also important to include key habitat building taxa such as scleractinian corals, calcifying algae and seagrass, and the future inclusion of threshold data from other taxonomic groups would improve confidence that thermal SSDs can adequately represent tropical marine communities.

4.2 Thermal stress SSD

The thermal threshold values in this dataset ranged from 1 to 7.9°C but there was no apparent taxonomic pattern driving differences in thermal tolerance. The thermal stress threshold has previously been shown to be linearly related to acclimation temperature across wider temperature ranges, with reduced *TT_x* for species observed for species acclimated at warmer temperatures (de Vries et al., 2008; McErlean et al., 1969). This is consistent with the *climate variability hypothesis* based on the decrease in annual SST variation range from temperate areas to the tropics, which results in coral reef ectotherms exhibiting smaller thermal windows and living closer to their thermal maxima (Compton et al., 2007; Stevens, 1989). Thus, it is likely that climate change is most stressful for tropical organisms. The experiments that

generated the toxicity thresholds for tropical species here applied acclimation values from 23°C to 29°C and these were not correlated with TTx (Figure 1:). It is possible that the lack of correlation was due to the relatively narrow range of Ta values, or that the dataset needed to be larger for this correlation to become clear. Nevertheless, the lack of relationship between TTx and Ta in this dataset allowed us to employ TTx values as temperature intervals (°C scale exceeding acclimation) on the x-axis of the SSD, so a single SSD could be directly applied across temperature acclimation scenarios (within the Ta range 23-29°C). Most experimental thermal stress experiments presumably acclimated the test species in the middle of their relative narrow thermal range, yet it is likely that acclimation at average summer maxima would yield even narrower TTx values as organisms will already be close to their upper thermal tolerance. This experimental approach may generate TTx values more compatible with other metrics for stress on coral reefs such as degree heating weeks (see below).

While 30 species were included in the SSD dataset, many of the threshold values were clustered between TTx 3 - 4°C, which may be influenced by often-large experimental temperature increments and a reliance on NOET to identify thresholds. More precise thresholds derived from modelling temperature responses (e.g. ET10) are likely improve the distribution of thresholds in future thermal SSDs. As well as being consistent with methods for deriving water quality guidelines, the use of ET10/NOET values is more inherently conservative than applying LT50 data (temperature above acclimation causing 50% mortality), which would instead generate an SSD that predicts proportions of the community seriously impacted (e.g. killed) by elevated temperatures. Thermal SSDs for mostly temperate aquatic species (freshwater and marine combined) have been previously generated using LT50 data (de Vries et al., 2008). That study found a linear relationship between LT50 and LT10 for 13 species of fish and bivalves and this relationship was applied to a larger number of species to derive a more protective thermal stress SSD based on LT10, similar to our tropical SSD (see below). Other thermal SSDs have been constructed for temperate freshwater fish (Leuven et al., 2011) and molluscs (Collas et al., 2018; Verbrugge et al., 2012) based on temperature ranges in the field and laboratory data. The use of thermal ranges from field data allowed the generation of SSDs to also assess the tolerance of fish and bivalves to low temperatures, an approach that could be adapted to predict latitudinal responses of coral communities as the climate changes.

4.3 Water temperature thresholds and temperature stress guidelines

The generation of a thermal stress SSD for tropical species from ET10/NOET data allowed us to derive thermal limits (e.g. PT95 = 1.2°C), below which a proportion (e.g. 95%) of the community would be protected from serious effects of thermal stress. This result is consistent with the HTI5 < 2°C (equivalent to our PT95) calculated by de Vries et al. (2008) for 50 temperate aquatic species based on 10% mortality data (similar to our TTx). While the protection temperature values we derived from the thermal SSD were calculated in the same way as water quality guidelines (Hobbs et al., 2005; Warne et al., 2018a), care should be taken before interpreting these PTx values as guidelines for direct application in a regulatory sense or for risk assessments. One of the key considerations is that exposure duration is not well addressed by the process of deriving water quality guidelines (Warne et al., 2018a). Water quality guidelines favour toxicity data from chronic exposures (typically ≥14 d for benthic

invertebrates and seagrass or shorter for early life stages such as fertilisation, larval development or microalgal growth) rather than acute exposure data. This constitutes a conservative approach allowing for maximum body burdens (hence maximum toxicity) to be reached (Warne et al., 2018a). For consistency and to enable combination of the thermal SSD with established water quality SSDs in ms-PAF, the thermal stress thresholds for each species in the SSD were also taken from chronic exposures as defined by Warne et al. (Warne et al., 2018a). However, when the upper thermal threshold is approached or exceeded, the negative impacts of thermal stress on marine ectotherms are cumulative, depending on both the intensity and duration of the exposure (Nguyen et al., 2011; Urban, 1994). The best-known example in tropical marine ecosystems is thermal bleaching of corals where photosynthetic symbionts are lost (often leading to colony mortality) during periods of high sea surface temperatures (SST), and the intensity of bleaching increases with duration of exposure to these conditions (Berkelmans, 2009; Hoegh-Guldberg, 1999). The analysis of many years of bleaching and SST data has led to the development of bleaching threshold indices such as Degree Heating Weeks (DHW), a measure of thermal stress accumulated through time, calculated by integrating temperatures at least 1°C above the mean monthly maximum (the historic value of the hottest month derived from a climatology) accumulated over the preceding 12 weeks (Liu et al., 2013). This was based on early findings that temperatures > 1°C above usual summer time maxima cause stress to corals (Glynn and D'Croz, 1990). For example, 4 weeks of temperatures 1.5°C above the mean monthly maximum equals 6 DHW (°C-weeks), and between 4 and 8 DHW have been shown to lead to widespread coral bleaching and habitat destruction in the tropics (Hughes et al., 2017b). Other field observations based on mortality curves (LT50) suggested that coral stress leading to bleaching and mortality can start earlier than 1°C above normal summer temperatures (Berkelmans, 2009). This accumulated thermal stress in corals which begins at 1°C above the normal field temperatures lies between the PT99 (0.58°C) and the PT95 (1.2°C), indicating the PTx values derived from the thermal stress SSD are within the appropriate ecological range for coral reefs. Thus, at least for the habitat forming corals, the SSD approach is consistent with DHW-based bleaching thresholds. The application of SSDs to define thermal risk is a promising approach and thermal stress SSDs should be further refined with data from experiments that model no effect temperature or ET10 values, are carried out over multiple exposure periods and address a wider range of taxa.

4.4 Using ms-PAF to estimate the influence of thermal stress on water quality guidelines

The application of chemical addition (assuming same mode of action) and response addition (different modes of action) models to predict the response of contaminant mixtures had been applied to individual species (de Zwart and Posthuma, 2005), and more recently to predict joint effects on aquatic communities by combining multiple SSD data using the ms-PAF method (Backhaus and Faust, 2012; Parkerton et al., 2018). Our study shows how the extension of ms-PAF to predict the simultaneous effects of contaminant and non-chemical stressors (in this case temperature) could be applied to adjust water quality guidelines to account for thermal stress. While the more direct approach of testing the toxicity of contaminants at many temperatures would be the preferred method to generate SSDs at thermally stressful temperatures, the datasets available are limited to few toxicants and taxa (see examples below). The contaminant SSDs developed at different temperatures have so far been generated for species exposed within their normal thermal windows (e.g. tropical vs temperate)

(Bejarano et al., 2017; Kwok et al., 2007; Raymundo et al., 2019; Zhou et al., 2014)), but do not generally account for the additional thermal stress as species encounter abnormally high SSTs. A benefit of the ms-PAF approach is that it can draw upon the many existing contaminant SSDs, and accounts for the additional thermal stress by the development of a thermal stress SSD to predict the influence of elevated temperatures on toxicity.

Combining the thermal stress and contaminant SSDs using the RA joint effect model resulted in reduced PCx values for copper and diuron as temperature increased, with for example reductions of between 41 and 82% (PC90) predicted at temperatures of 1.5°C above normal acclimation temperatures. Thus, even under the ambitious goals of the Paris agreement (UNFCCC, 2015), and definitely under more realistic scenarios (Collins et al., 2013) this study illustrates that contaminant guideline thresholds will need to be adjusted. At 1°C above normal acclimation temperatures, adjustment to the guideline values would be in the 7 - 59% range, while the PC99 for copper and diuron would be reduced by 67 and 23% respectively at 0.5°C above normal acclimation (and may be applicable during current high SST anomaly events). These reductions in predicted concentrations of copper and diuron to reach guideline values are not large in scale because the temperature ranges being considered are relatively small (albeit ecologically relevant). As the temperatures increase to over 2.4°C above acclimation it is expected (from the thermal SSD) that more than 50% of the tropical reef community would have reached the thermal threshold, so temperature itself would dominate negative effects on the community.

4.5 Validating the ms-PAF approach to predict the influence of thermal stress on contaminant toxicity

There are few laboratory data that can be used to effectively validate the ms-PAF approach taken here, apart from comparing the scale of toxicity change in contaminant SSDs that have been generated at different temperatures (e.g. temperate vs tropical) and the results of single species ecotoxicology tests for copper and diuron conducted using multiple temperatures. One of the most interesting comparisons is with a meta-data analysis of temperate vs tropical freshwater SSDs made for 18 contaminants (Kwok et al., 2007). In that study, PC90 (HC10) values were separately generated for tropical and temperate species, where experiments were conducted within their normal temperature ranges. Those ranges differed by a median value of 5.7°C. The PC90 ratios of temperate/tropical from those datasets ranged from 0.013 to 16.2. This indicates that guidelines for tropical species cannot be readily derived or converted from temperate species SSDs (sometimes over estimating and sometimes underestimating toxicity). Another recent study derived SSDs for three metals from multiple single temperature tests (performed at different temperatures) and showed reductions in PC90 values by almost 50% across +2°C intervals (Zhou et al., 2014). These studies and others that compare differences in sensitivity between temperate and tropical communities generally recommend a 10-fold reduction (safety factor) to be applied to water quality guidelines to account for these large differences in PC90 values (Lau et al., 2014). It should be noted that most of these comparisons between temperate and tropical SSDs have been made from datasets that do not account for thermal stress. Instead the differences in toxicity are attributed to contaminant type, toxicokinetics at different temperatures and species composition (in each SSD). Those studies show that water quality guidelines should take into account regional climatic conditions

and species compositions, and the ms-PAF approach presented here extends this approach by adjusting guidelines developed from regionally relevant SSDs for abnormally high SSTs.

More specific validation of the ms-PAF predictions can be made by comparison with single species copper and diuron toxicity tests on tropical marine species, conducted at different temperatures. The effects of simultaneous copper and thermal stress on adult corals and larvae have been assessed in several studies, but most were conducted within the normal temperature range (3°C) of the species tested and the elevated temperature had only minor influences on copper toxicity (da Silva Fonseca et al., 2017; Kwok et al., 2016; Kwok and Ang Jr, 2013). When a wider temperature range was tested, there were strong individual and combined effects of thermal stress and copper on larval settlement of the corals *Acropora millepora* and *A. tenuis* (Negri and Hoogenboom, 2011). In those experiments, the EC50s for copper exposure reduced by 27% and 19% at +3°C above acclimation. That same dataset was assessed using the RA model of joint action (Uthicke et al., 2016), demonstrating the combined effects of most combinations of copper and temperatures up to +3°C above acclimation were accurately predicted by the RA model (indicating additivity), while combinations of copper and +4°C were more toxic than predicted (indicating a synergistic interaction). Although this was the only previous study to apply the RA model to copper and temperature exposures, it demonstrates that for two coral species the RA model of joint action can be effective for estimating the combined effects of thermal stress and copper (for up to +3°C above acclimation) and is quantitatively consistent with the choice of the RA model in the ms-PAF in the present study.

The toxic effects of the herbicide diuron to tropical species also increases at elevated temperatures. Photosystem II herbicides (diuron, atrazine and hexazinone) and thermal stress inhibited photosynthetic efficiency led to bleaching in the coral *Acropora millepora* both independently and in combination across a 6°C temperature range (Negri et al., 2011a). The effects were additive (there was no interaction between temperature and diuron between these stressors over the range), indicating RA should be a valid joint effects model for this species. The RA model has since been used to assess the joint action of temperature and diuron to tropical coral symbionts, symbiont-bearing foraminifera and seagrass. The effects of temperature and diuron on photosynthetic efficiency was predicted using the RA model to within 20% of the observed effects in two species of cultured dinoflagellate symbionts *Cladocopium* sp. and *Durusdinium* sp. (formerly *Symbiodinium* Clade C1 and D) (van Dam et al., 2015), four species of tropical symbiont bearing foraminifera (*Heterostegina depressa*, *Marginopora vertebralis*, *Calcarina mayorii* and *Alveolinella quoyi*) (van Dam et al., 2012) and the tropical seagrass *Halophila ovalis* (Wilkinson et al., 2017), further validating this approach for assessing the response of multiple stressors.

The RA model of joint action assumes the stressors have different modes of action and do not interact with each other (de Zwart and Posthuma, 2005). While it is highly likely that these contaminants and temperature do interact (influencing bioavailability and toxicokinetics (Cairns et al., 1975)), these interactions may be minor at the low-level combinations of contamination and thermal stress that are relevant to climate adjustments of water quality guidelines (which have been calculated from NOEC, NOET, EC10 and ET10 data). It is evident from the small number of single species multi-stressor experiments described above that the RA model can be suitable for predicting joint effects of low-level stressor combinations that include temperature. Reviews of the effectiveness of both the CA and RA models to predict the impacts

of multiple chemicals on aquatic organisms have revealed good agreement with observed responses, and cases of underestimation (due to synergistic effects) are rare (Belden et al., 2007; Cedergreen et al., 2008). However, it is still possible for the RA and the CA models to underestimate impacts (synergistic effects are not predictable), and further validation of this approach is needed across a far wider range of species and combinations of chemical and thermal.

4.6 Applying ms-PAF to report, regulate and manage pollution and thermal stress on coral reefs

Further development of the ms-PAF approach of predicting the combined effects of thermal stress and contaminants on tropical reef communities has several related applications for reporting, regulating and monitoring coral reefs. These include: (i) developing temperature/climate-adjusted water quality guidelines for single contaminants; (ii) quantifying maximum pollution concentrations to maintain the resilience of coral reefs to thermal stress events including bleaching and (iii) evaluating monitoring data to account for combined risks posed by simultaneous exposure to pollutants and thermal stress towards more comprehensive environmental reporting and assessments.

In this study we explored the process of applying the ms-PAF method to predict the influence of additional temperature stress on the toxicity of copper and diuron. The water quality guidelines (previously referred to as trigger values) are primarily used as benchmark values to guide the protection of marine communities or ecosystems. To maintain the desired level of protection, for example 99% of all species, during a heatwave the PC99 for the contaminant could be adjusted according to Table 2, where T_a is equivalent to the temperature above the normal monthly average. Similar adjustments could be made to all water quality guidelines where SSDs are available for incorporation into the ms-PAF method.

A similar approach could be taken to quantify the influence of water quality on heat stress to coral reef communities. For example, if a thermal stress SSD predicts 10% of the community could be affected over prolonged heating of 1.6°C above the historical summer SST (=PT90), then from ms-PAF it is predicted from Table 2 that any copper or diuron contamination over the PC99 values of 0.29 and 0.43 $\mu\text{g L}^{-1}$ respectively would rapidly increase the proportion of the community affected. This approach could be customised for assessing multi-stressor risks of coral bleaching by the development of coral only SSDs (potentially populated with both field and laboratory data). Compatibly with current metrics for bleaching risk (DHW) would also be improved by substituting the acclimation temperature (T_a) with the maximum monthly temperature (T_{max}) and encouraging future experimental work to prioritise this approach. ms-PAF could also be applied to assess risk spatially and temporally by including thermal stress and contaminants as exposure layers in models and using in SSDs and ms-PAF to model the potentially affected fractions of communities from individual locations and points in time.

Assessing the risk posed to a community by complex mixtures of contaminants that coincide with an abnormal heating event can be assessed firstly by identifying the chemical and non-chemical stressors (i.e. thermal stress) that co-occur and their expected exposures from modelling or monitoring data. ms-PAF can then be applied in two steps to account for the effects of single stressors that co-occur, firstly by applying CA model to calculate the total PAF

for contaminants with the same mode of action, then by applying the RA model to account for the effects of stressors with different modes of action. This results in a single risk metric expressed as the potentially affected fraction of the community to the modelled or measured multi-stressor exposures. The inclusion of the physical stressor temperature is an extension of the mixed model ms-PAF approach proposed by de Zwart and Posthuma (2005) and applied to complex chemical mixtures, including those with up to 10 different modes of action (Parkerton et al., 2018) and those being applied to pesticide mixtures the Great Barrier Reef in ecosystem monitoring and reporting programs (Waterhouse et al., 2018).

5.0 CONCLUSION AND FUTURE DIRECTIONS

The generation of a thermal SSD for benthic marine organisms relevant to coral reefs presents an additional option for interpreting and quantifying the hazards posed by abnormally high SST that will become more frequent as the climate changes. Even under the very optimistic Paris targets of 1.5 and 2.0°C, increase in air temperature compared to pre-industrial levels, SST will increase a further 0.3 or 0.7°C, respectively (Magnan et al., 2016); whereas present trajectories point more towards further SST increases > 1.2°C. Thus, the need for climate adjusting water quality guidelines is urgent. This first thermal SSD for tropical marine species can be improved by the inclusion of additional existing data (experimental and field), and by modifying future experimental designs to include acclimation temperatures closer to summer maxima and smaller increments in temperature for more meaningful and precise calculation of thermal stress thresholds. Nevertheless, the preliminary thermal stress SSD generates plausible community protection values that can be considered application in multi-stress risk assessments. However, we also note that our SSD confirms that a large fraction of the species complement on coral reefs is threatened by temperature increase alone.

Understanding the combined hazards and risks posed by multi-contaminant mixtures is a developing field, with ms-PAF being one of the most widely explored “bottom-up” methods (Beyer et al., 2014). The extension of ms-PAF to include thermal stress is a promising approach that could enable the rapid development of climate-adjusted water quality guidelines, and quantification of pollution targets to help manage and protect coral reefs from thermal stress events. Following further refinements of the thermal stress SSD and validation of ms-PAF model choice, additional non-chemical stressors could be included. The development of SSDs for ocean acidification (Azevedo et al., 2015; de Vries et al., 2013), sediment exposures (Smit et al., 2008), anoxia (Elshout et al., 2013), and salinity (Kefford et al., 2011; Verbrugge et al., 2012) are already underway and offer further options to advance more comprehensive environmental guidelines, reporting and assessments.

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APPENDIX 1: SCORING SYSTEM FOR ASSESSING QUALITY OF TOXICITY DATA

Table 3: Scoring system for assessing the quality of toxicity data for non-metals to freshwater non-plants to be used in the derivation of guideline values for toxicants (modified from Hobbs et al. 2005, Warne et al., 2018a).

No.	Question	Answer Options		
1	Were the acclimation conditions measured and stated? (<i>Environmental conditions at time of collection or laboratory culture conditions</i>)			
1.1	Temperature	Measured & stated (5)	Only stated (2)	Not measured or stated (0)
1.2	Light intensity	Measured & stated (2)	Only stated (1)	Not measured or stated (0)
1.3	Dissolved Oxygen	Measured & stated (2)	Only stated (1)	Not measured or stated (0)
1.4	pH	Measured & stated (2)	Only stated (1)	Not measured or stated (0)
1.5	Conductivity/Salinity	Measured & stated (2)	Only stated (1)	Not measured or stated (0)
1.6	Was the period of laboratory acclimation stated? (time before test that organism acclimated to baseline conditions)	Period stated (5)	Not stated (0)	
2	Incremental rate of change in temperature from acclimation to test conditions			
2.1	Was there an incremental change in temperature from acclimation temperature to test temperature and was this rate of change stated/inferred? (e.g. temperature increased from 25 to 30 degrees in 0.5 degree increments over a period of 'x' hours).	Incremental change and rate of change stated/inferred (10)	Non-incremental change and rate of change inferred OR incremental change and rate of change not stated/inferred (5)	No-incremental change and rate of change not stated/inferred (0)
2.2	What was the temperature increment?	≤ 1°C (5)	2°C (3)	>2-5°C (1) ≥ 5°C (0)
3	Was the test duration stated/inferred? (e.g. 48h, 96h, etc.) Note: <u>Data that fail this question are automatically deemed to be of unacceptable quality and must not be used.</u>	Stated (10)	Inferred (5)	Not stated or inferred (0)
4	Were appropriate controls used? Note: <u>Data that fail this question are automatically deemed to be of unacceptable quality and must not be used.</u>	Yes (5)	No (0)	
5	Was each control treatment at least duplicated? Note: <u>Data that fails this question cannot be of high quality.</u>	Yes (5)	No (0)	
6	Were test acceptability criteria stated OR were there ≤10% effect to control organisms and was the variability around the control mean acceptable? Note: <u>Data that fail this question/acceptability criteria are automatically deemed to be of unacceptable quality and must not be used.</u>	Stated (10)	Acceptable control effect/mean variability (5)	Not stated or inferred (0)
7	Were the characteristics of the test organism/s (length, mass, age, etc.) stated?	Yes (5)	No (0)	
8	Was the type of test media used stated?	Yes (5)	No (0)	
9	Was the biological endpoint stated and defined (e.g. mortality, population growth, etc.)?	Stated and defined (10)	Stated (5)	Not stated (0)
10	Was the biological effect stated (LC or NOEC)?	Yes (5)	No (0)	

11	Was the biological effect quantified (e.g. 50% effect, 25% effect, etc.)?	Yes (5)	No (0)		
12	During the test period was the media temperature measured? Note: <u>If media temperatures were not measured then automatically the data cannot be of high quality.</u>	More than twice (5)	Twice (3)	Once (1)	Not measured (0)
13	Was the media temperature measured directly or indirectly? Directly = Temperature probe Water bath, temperature controlled room, etc. Indirectly = Note: <u>If media temperatures were not measured then automatically the data cannot be of high quality.</u>	Directly (5)	Indirectly (2)	No (0)	
14	Was a temperature response relationship either observable or stated?	Yes (4)	No (0)		
15	Was an appropriate statistical method or model used to determine effect or significant difference from control? Note: <u>Data that fail this question are automatically deemed to be of unacceptable quality and must not be used.</u>	Yes (5)	No (0)		
16	For LC/EC/BEC data was an estimate of variability used OR for NOEC/LOEC data was the significance level 0.05 or less? Note: <u>Data that fail this question are automatically deemed to be of unacceptable quality and must not be used.</u>	Yes (5)	o (0)		
17	Were the following test parameters measured and stated?				
17.1	Light intensity	Measured twice or more (3)	Measured once (2)	Only stated (1)	Not measured or stated (0)
17.2	Dissolved Oxygen	Measured twice or more (3)	Measured once (2)	Only stated (1)	Not measured or stated (0)
17.3	pH	Measured twice or more (3)	Measured once (2)	Only stated (1)	Not measured or stated (0)
17.4	Conductivity/Salinity	Measured twice or more (3)	Measured once (2)	Only stated (1)	Not measured or stated (0)
18	Were the following test light conditions specified?				
18.1	Photoperiod?	Yes (3)	No (0)		
18.2	Light source (natural, shaded, artificial light, etc.)?	Yes (3)	No (0)		
18.3	Mean maximum daily light intensity?	Yes (3)	No (0)		

Total possible score = 138

Quality score: [Total score/Total possible score] x 100

H = high quality

A = acceptable quality

U = unacceptable quality

Quality score of ≥80%

Quality score of >50% to <80%

Quality score ≤50%

Table 4: Species sensitivity distribution parameters for the Burr type III distribution calculated for the thermal stress, diuron and copper datasets using BurrIoz 2.0 software (CSIRO, 2019).

	b	c	k	R ²
Thermal stress	4.65422	5.13843	0.43006	0.967
Diuron	-0.75178	0.27332	1.81746	0.980
Copper	11.93875	0.63686	1.87726	0.983

