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Supplementary Materials for

Metabolomic shifts associated with heat stress in coral holobionts

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The PDF file includes:

Figs. S1 to S6
Tables S1 and S2
Legends for data files S1 and S2

Other Supplementary Material for this manuscript includes the following:

(available at advances.sciencemag.org/cgi/content/full/7/1/eabd4210/DC1)

Data files S1 and S2

Figure S1. Metabolomic analysis of Hawaiian corals. (A) Accumulation pattern of metabolites in *M. capitata* at different unadjusted significance levels from T1-T5 under ambient and thermal stress conditions. (B) Montiporic acids identified in the coral holobiont. (C) Accumulation of different MAs in *M. capitata* (MC) and *P. acuta* (PC) in samples collected from the field.

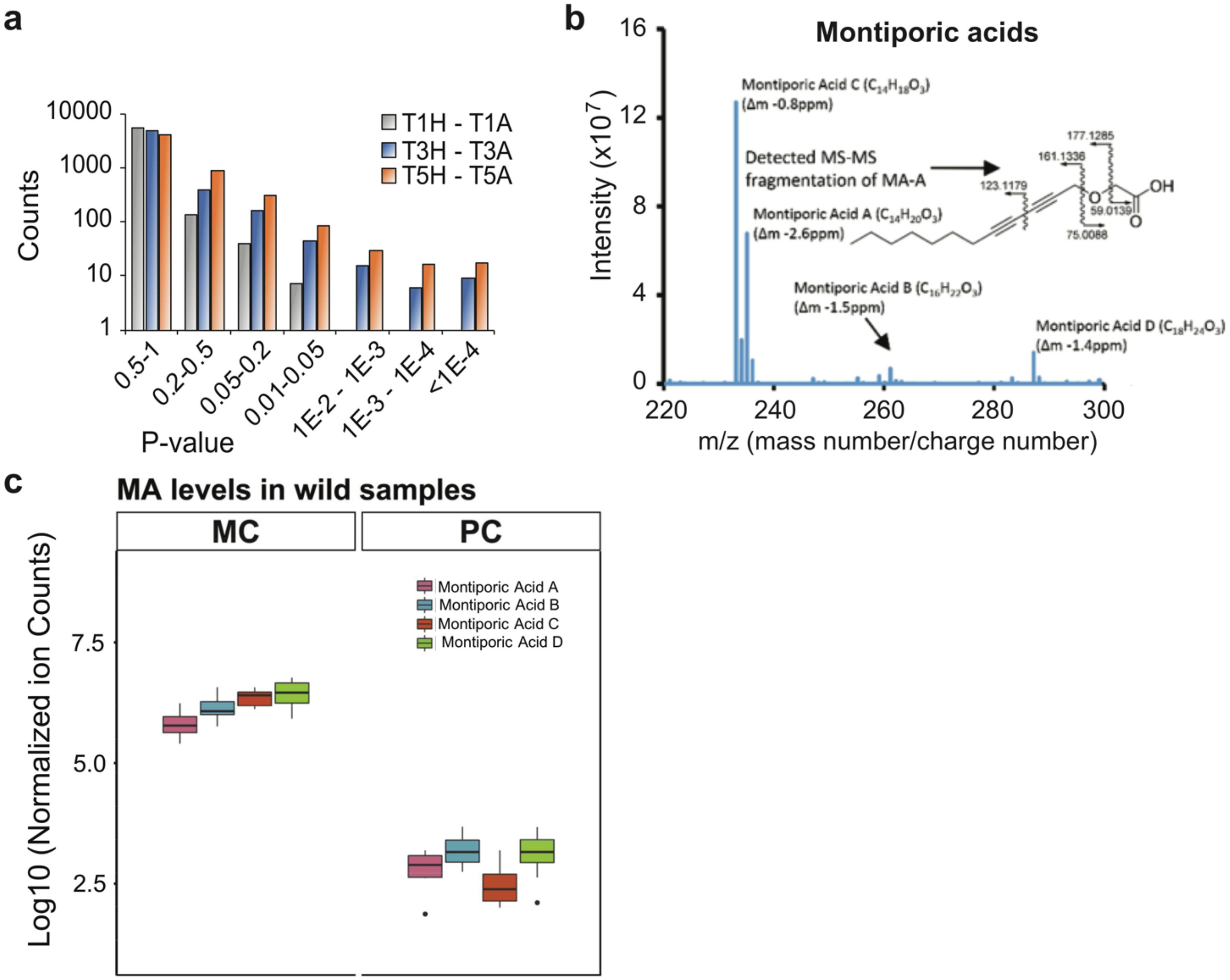

Figure S2. Visualization of the complete *Montipora capitata* (A) and *Pocillopora acuta* (B) polar metabolite data. These Log-Log plots show the relative intensity of features included in the total data set. The figure quartiles are the median signal intensity of the ambient samples and the median signal intensity of the high samples for each metabolite. The relative intensities of montiporic acids, amino acids, and dipeptides are highlighted.

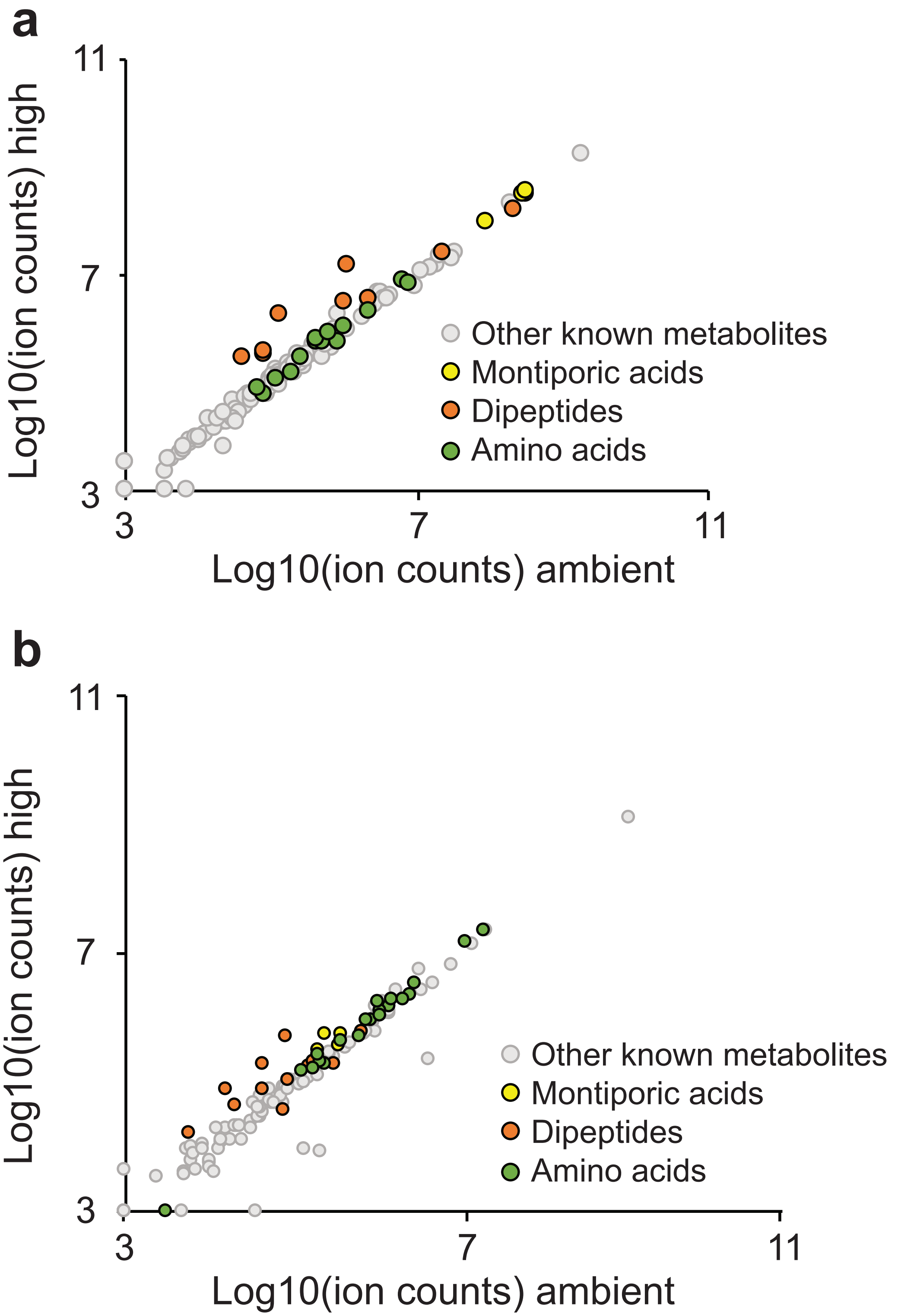

Figure S3. Volcano plots of metabolites generated from *P. acuta* and *Aiptasia* under positive ionization mode. (A) Analysis of *P. acuta* data under ambient and high temperature treatments at the three sampling points. (B) Analysis of *Aiptasia* under symbiotic and aposymbiotic (alga free) conditions. Putative dipeptides are shown with the filled brown circles in all plots.

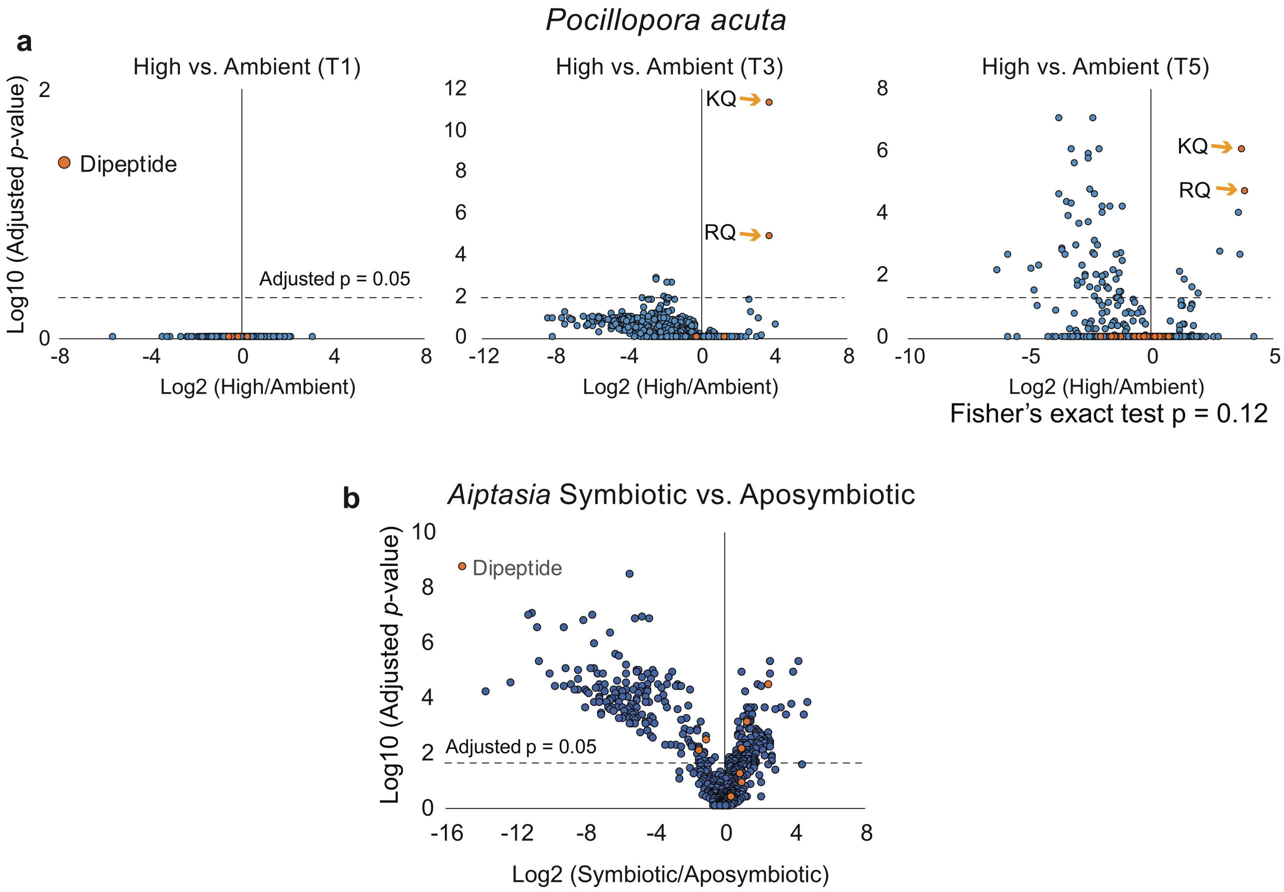

Figure S4. Dipeptide production by stony corals under thermal stress (T1-T5). (A-D) Normalized ion counts of dipeptides RQ, KQ, RV, and RA under heat stress in three nubbins from the four individual colonies that we studied (206, 248, 289, 291, respectively). Note that colony-by-colony, as well as nubbin-by-nubbin variation, although the overall ion count changes are significant (Figs. 1, 2).

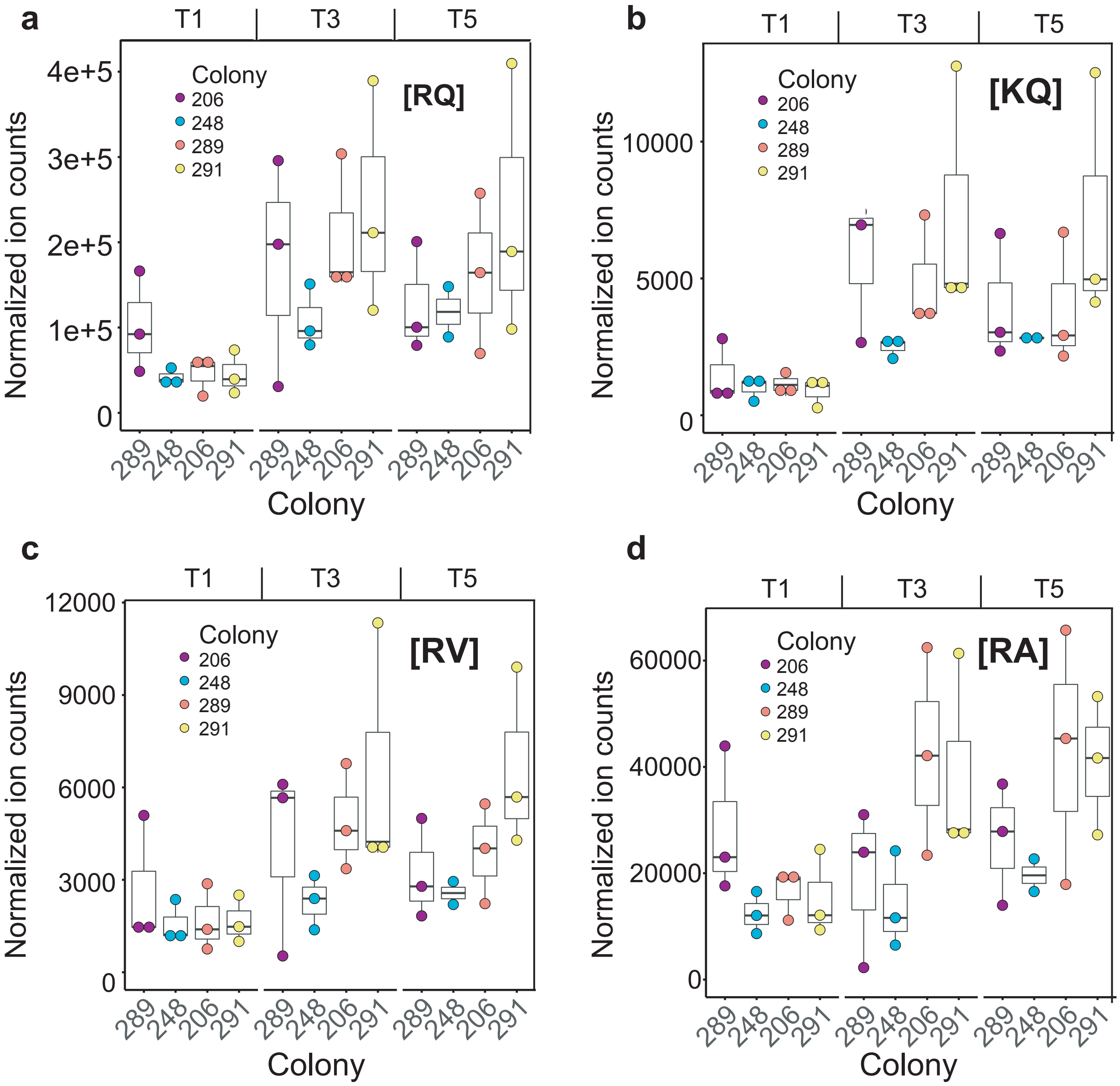

Figure S5. Annotated network of metabolite co-occurrence in *M. capitata* at T5. (A) Ambient treatment network and (B) thermal stress network. Dipeptides are shown as triangles (under both positive and negative ionization modes) and other metabolites as circles with annotations, when available. Metabolite intensity and type of correlation are shown in the legend.

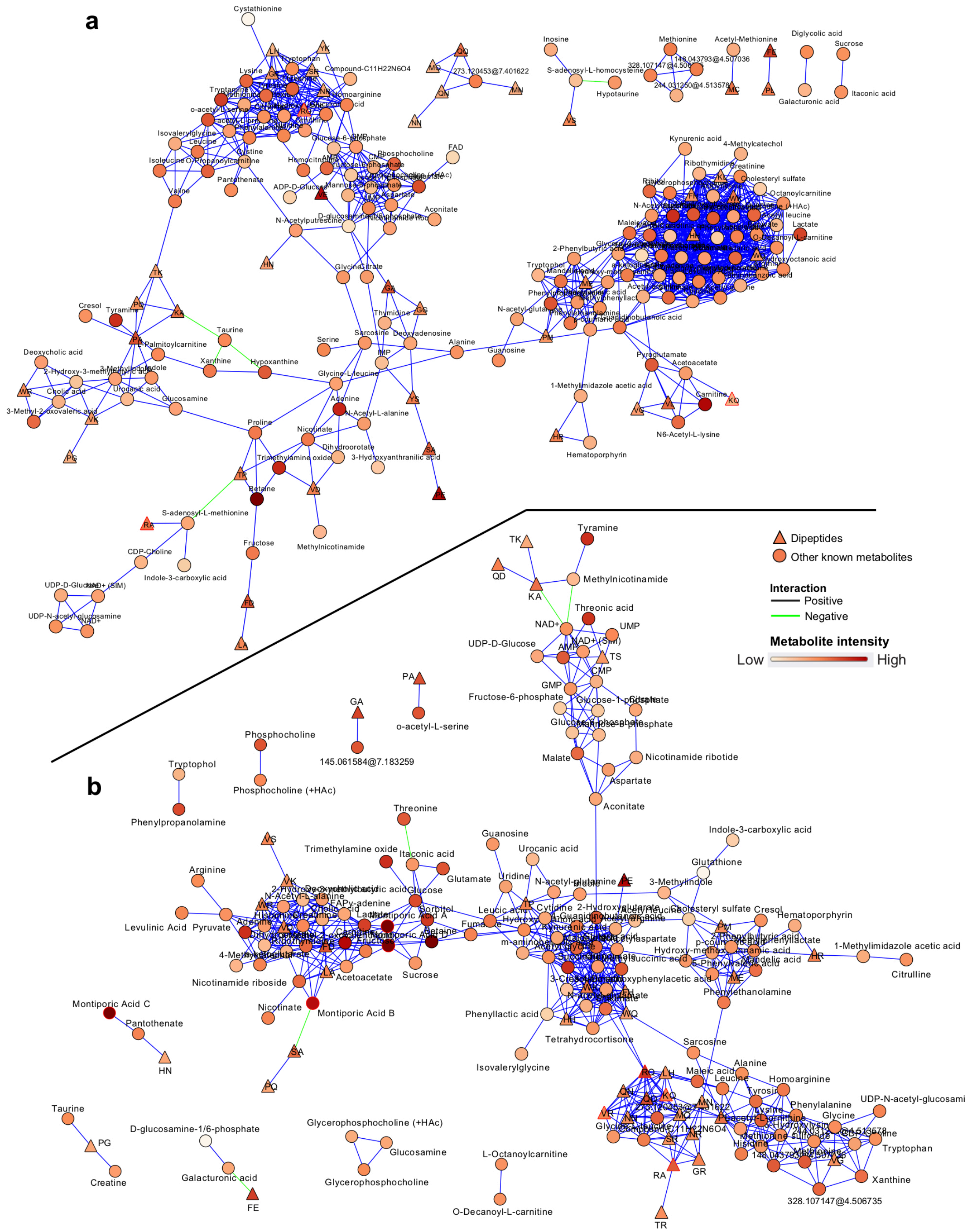

Figure S6. Analysis of metabolites in *Aiptasia*. (A) Metabolite (RQ) amount in symbiotic and aposymbiotic *Aiptasia* samples. (B) Metabolite (KQ) amount in symbiotic and aposymbiotic *Aiptasia* samples. (C) Metabolite (RV) mount in symbiotic and aposymbiotic *Aiptasia* samples. (D) Metabolite (RA) amount in symbiotic and aposymbiotic *Aiptasia* samples.

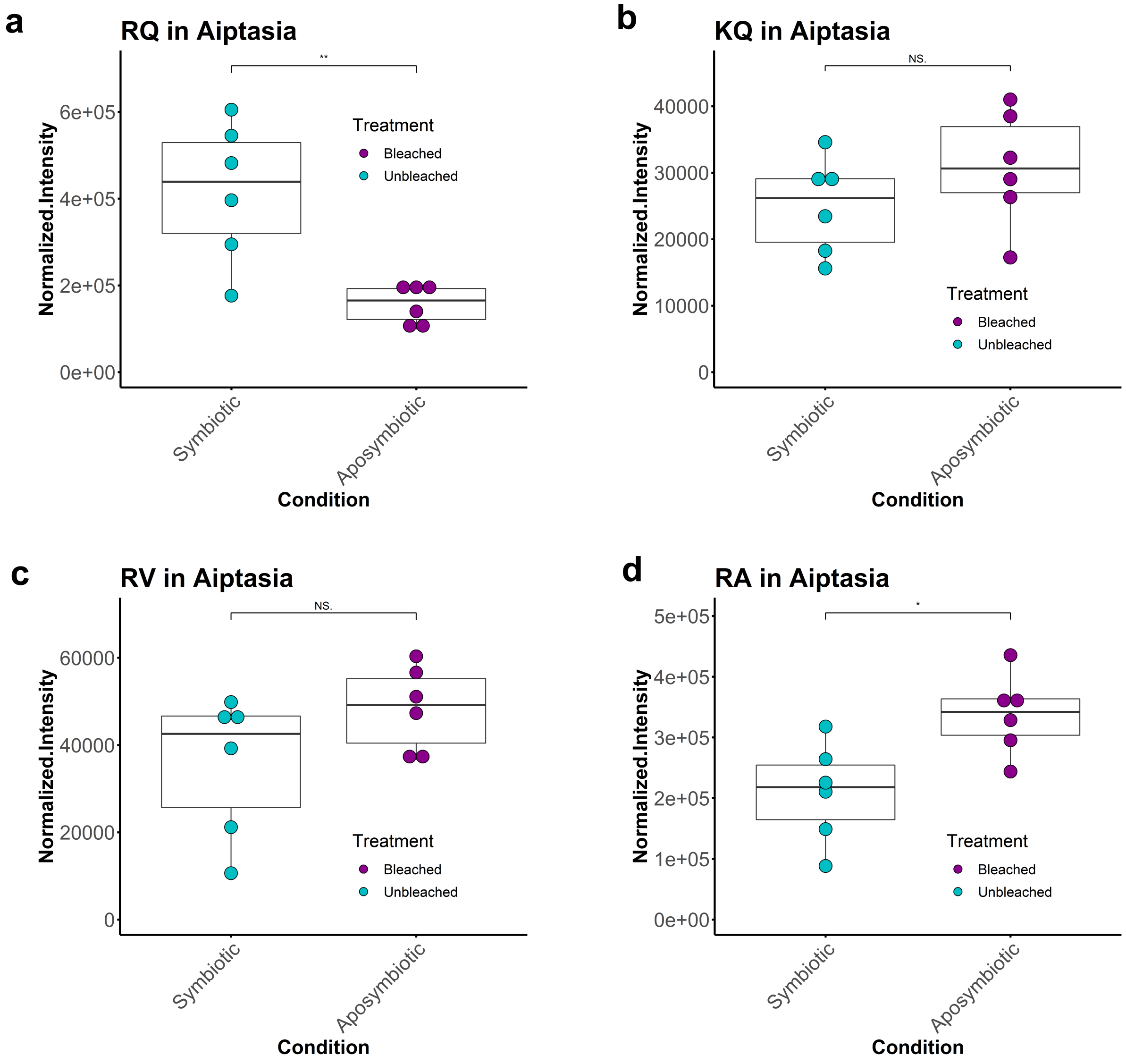

Table S1.

Coral peptide identification by retention time and MS^2 spectra matching.

Coral Dipeptide	Peptide Standard	RT (min)	ΔRT (min)	MS^2 Spectra Matching
$C_{11}H_{22}N_6O_4$ (RT 9.05min)	**RQ**	**9.1**	**0.05**	**99.69%**
	QR	8.82	-0.23	85.33%
	ER-NH2	9.38	0.33	77.86%
	RE-NH2	9.3	0.25	97.36%
	γ-ER-NH2	10.84	1.79	86.41%
	AGR	8.71	-0.34	86.95%
	RAG	8.62	-0.43	96.64%
	RGA	8.62	-0.43	96.83%
$C_{11}H_{22}N_4O_4$ (RT 9.96min)	**KQ**	**9.98**	**0.02**	**99.15%**
	QK	9.54	-0.42	82.35%
	EK-NH2	10.21	0.25	91.62%
	KE-NH2	10.11	0.15	99.46%
	γ-EK-NH2	12.89	2.93	98.23%
$C_{11}H_{23}N_5O_3$ (RT 7.64min)	**RV**	**7.62**	**-0.02**	**98.12%**
	VR	6.81	-0.83	54.50%
$C_9H_{19}N_5O_3$ (RT 8.97min)	**RA**	**8.95**	**-0.02**	**99.36%**
	AR	8.98	0.01	86.19%

Table S2.

Average dipeptide by community (ADPC) scores for dipeptides in the networks derived from the *M. capitata* lab manipulations. AMB is the ambient condition and HIT is the thermal stress treatment.

Conditions	Time	ADPC	#Community	DP	OKM	#Nodes	#Edges	Density	Centralization
AMB	T1	0.2599559	25	34	121	155	309	0.0259	0.066
AMB	T3	0.2573268	11	45	170	215	2131	0.0926	0.156
AMB	T5	0.3119065	15	45	156	201	933	0.0464	0.135
HIT	T1	0.3071103	14	46	160	206	1012	0.0479	0.099
HIT	T3	0.2425315	18	42	147	189	571	0.0321	0.069
HIT	T5	0.2251791	16	42	138	180	639	0.0396	0.072

Data S1. Untargeted metabolomic data under positive and negative ionization modes and its characteristics from *M. capitata*, *P. acuta*, and *Aiptasia*.

Data S2. Targeted metabolomic data under positive and negative ionization modes and its characteristics from *M. capitata*, *P. acuta*, and *Aiptasia*.