

Supplementary Information

The interaction between the proliferating macroalga *Asparagopsis taxiformis* and the coral *Astroides calycularis* induces changes in microbiome and metabolomic fingerprints

Stéphane Greff[†], *Tânia Aires*[#], *Ester A. Serrão*[#], *Aschwin H. Engelen*[#], *Olivier P. Thomas*^{†,⊥,§},
Thierry Perez^{†,*}

[†] Institut Méditerranéen de Biodiversité et d'Ecologie marine et continentale, IMBE UMR 7263 CNRS / IRD / Aix Marseille Université / Avignon Université. Station Marine d'Endoume, rue de la Batterie des Lions, 13007 Marseille, France.

[⊥] GEOAZUR, UMR 7329 CNRS / Université de Nice Sophia Antipolis, Faculté des Sciences, Parc Valrose 06108, Nice, France.

[§] Marine Biodiscovery, School of Chemistry, National University of Ireland Galway. University Road, Galway, Ireland.

[#] CCMAR-CIMAR Centre for Marine Sciences, University of Algarve, Campus de Gambelas, 8005-139 Faro, Portugal.

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Table S2 – *Asparagopsis taxiformis* ions responsible for group 2 difference in the Principal Component Analysis (Fig. 6 in main manuscript). RT: Retention time in minutes, mS: mSigma is a constructor quality value of the formula determination. It compares accurate masses and isotopic patterns of experimental formula with theoretic ones (value of mSigma closest to zero are representative of maximal fit). Base peaks chromatograms were considered for ion formula determination.7

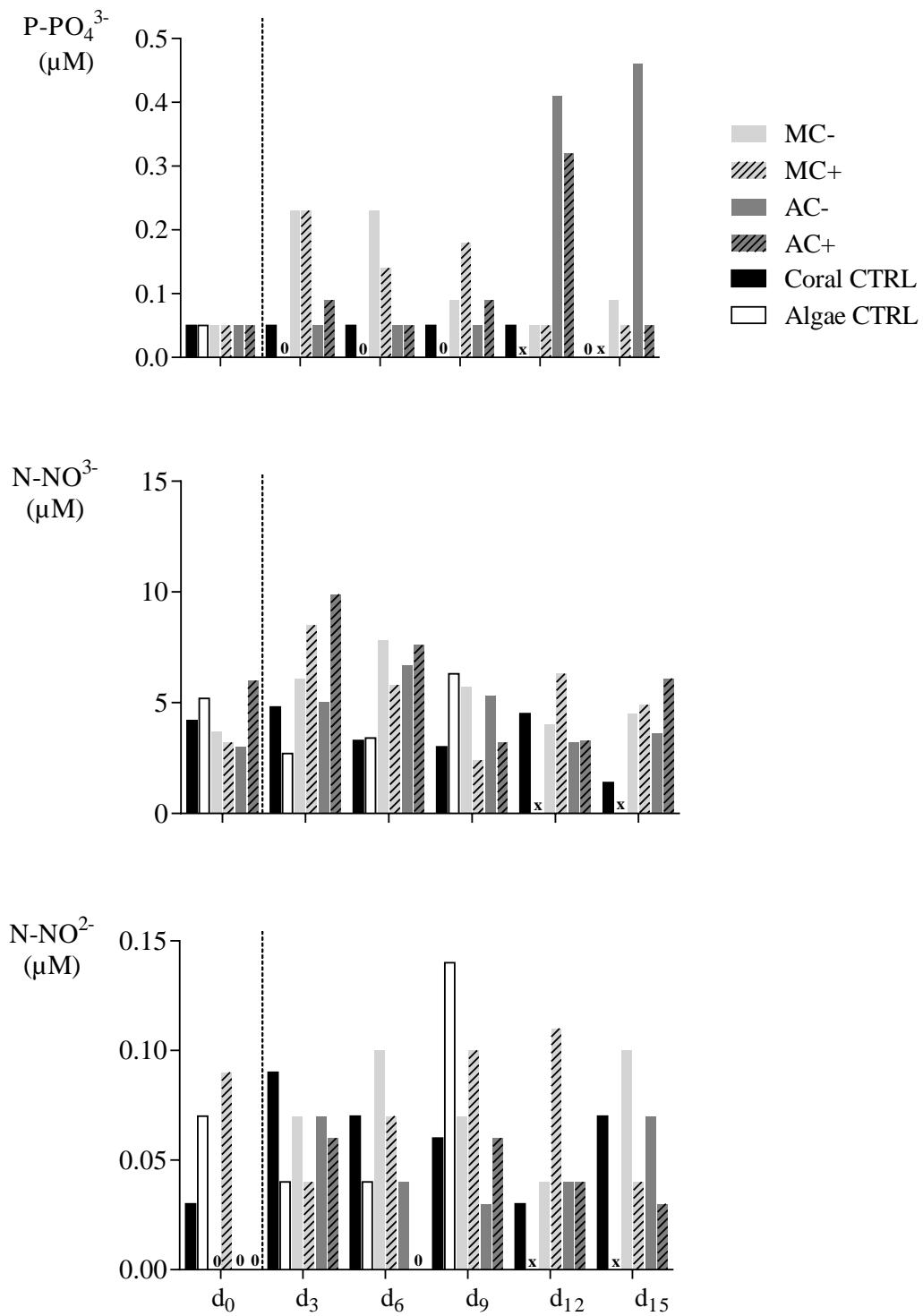


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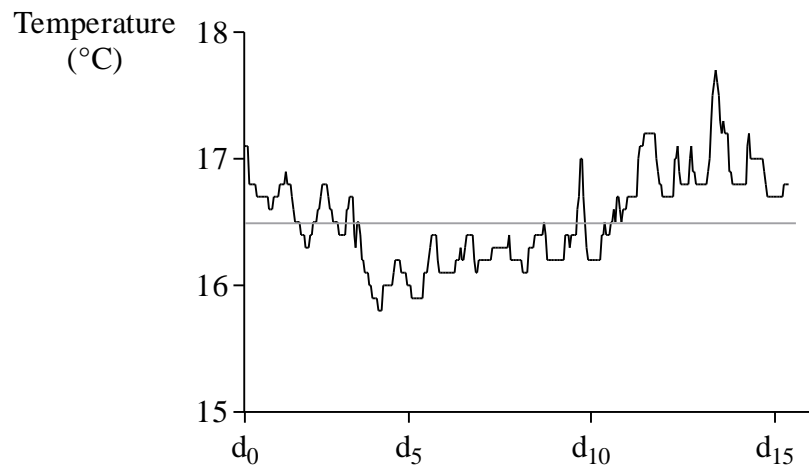


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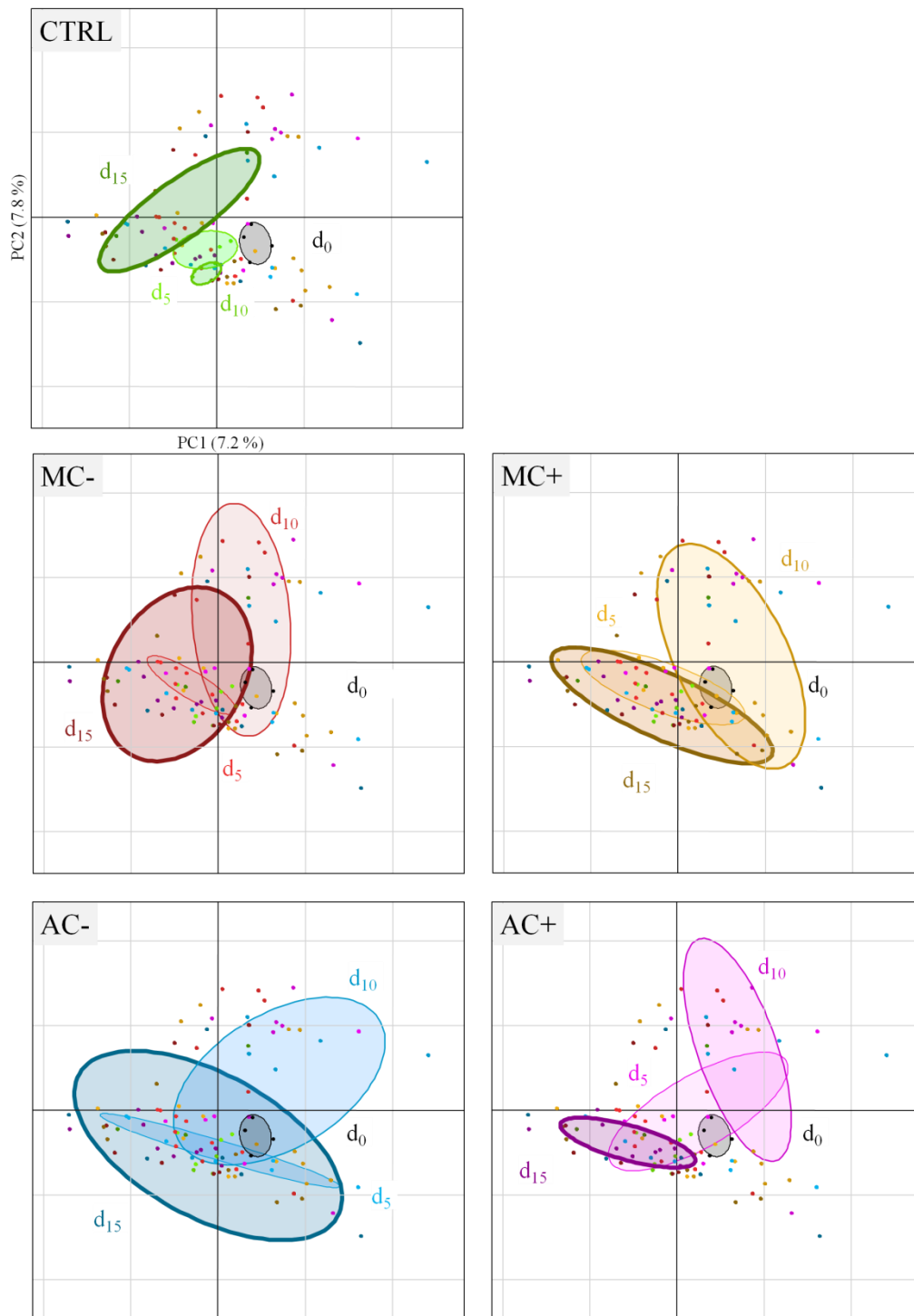


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Peak	RT (min)	BPC Area (%)	[M+H] ⁺	Ion formula	Annotation	mS
1	0.54	16.8	235.1650	C ₁₀ H ₂₃ N ₂ O ₄	-	1.2
2	0.57	8.6	387.1775	C ₁₈ H ₂₃ N ₆ O ₄	dihydrogenated orthidine (?)	3.2
3	0.86	0.6	387.1774	C ₁₈ H ₂₃ N ₆ O ₄	dihydrogenated orthidine (?)	13.6
4	2.83	20.2	194.0923	C ₉ H ₁₂ N ₃ O ₂	tubastrine	0.7
5	4.39	2.7	385.1619	C ₁₈ H ₂₁ N ₆ O ₄	orthidine	4.9
6	4.69	2.1	385.1617	C ₁₈ H ₂₁ N ₆ O ₄	orthidine	10.0
7	4.83	3.0	385.1619	C ₁₈ H ₂₁ N ₆ O ₄	orthidine	4.9
8	4.94	2.0	385.1618	C ₁₈ H ₂₁ N ₆ O ₄	orthidine	7.2
9	5.50	1.4	537.2716	C ₃₀ H ₃₃ N ₈ O ₂	-	13.2
10	5.83	2.1	537.2718	C ₃₀ H ₃₄ N ₈ O ₂	-	7.2
11	6.04	2.8	255.1235	C ₁₄ H ₁₅ N ₄ O	aplysinsin	3.6
12	6.12	19.1	269.1390	C ₁₅ H ₁₇ N ₄ O	<i>N</i> -methylaplysinsin	2.7
13	6.48	0.2	212.1755	C ₁₁ H ₂₂ N ₃ O	-	4.0
14	6.84	2.0	333.0339	C ₁₄ H ₁₄ BrN ₄ O	6-bromoaplysinsin	3.9
15	6.91	10.4	347.0495	C ₁₅ H ₁₆ BrN ₄ O	6-bromo- <i>N</i> -methylaplysinsin	18.3
16	7.09	0.9	311.1498	C ₁₇ H ₁₉ N ₄ O ₂	<i>N</i> -propionylaplysinsin	14.1
17	7.14	0.4	325.1654	C ₁₈ H ₂₁ N ₄ O ₂	<i>N</i> -methyl- <i>N</i> -propionylaplysinsin	19.5
18	7.34	0.5	524.2406	C ₂₉ H ₃₀ N ₇ O ₃	-	9.3
19	8.62	0.4	198.1848	-	-	-
20	8.84	2.9	214.0892	-	-	-
21	8.90	0.4	249.2058	-	-	-
22	10.87	0.3	440.4097	C ₂₇ H ₅₄ NO ₃	-	3.9

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RT (min)	positive mode				negative mode			
	[M+H] ⁺	Ion formula	Error (ppm)	mS	[M-H] ⁻	Ion formula	Error (ppm)	mS
3.3	-	-	-	-	186.1137	C ₉ H ₁₆ NO ₃	-0.9	3.7
3.9	-	-	-	-	168.1033	C ₉ H ₁₄ NO ₂	-1.7	7.1
4.0	-	-	-	-	214.1454	C ₁₁ H ₂₀ NO ₃	-2.6	5.1
5.8	288.2895	C ₁₇ H ₃₈ NO ₂	0.7	6.1	-	-	-	-
7.3	318.2401	C ₁₆ H ₂₈ N ₇	0	12.3	-	-	-	-
7.8	320.2562	C ₁₆ H ₃₀ N ₇	-1.2	1.2	-	-	-	-
8.0	280.2635	C ₁₈ H ₃₄ NO	-0.1	7.1	-	-	-	-
8.2	228.2321	C ₁₄ H ₃₀ NO	0.3	3.2	-	-	-	-
9.7	256.2634	C ₁₆ H ₃₄ NO	0.5	6.8	-	-	-	-
9.8	280.2631	C ₁₈ H ₃₄ NO	1.5	8.4	-	-	-	-
10.5	282.2790	C ₁₈ H ₃₆ NO	0.4	6.2	-	-	-	-
10.9	270.2793	C ₁₇ H ₃₆ NO	-0.8	2.4	-	-	-	-
12.6	284.2945	C ₁₈ H ₃₈ NO	1.0	11.4	-	-	-	-