Supplementary Material - Thesis

Chapter 2

Table S2.1: Fv/Fm values for *B. minutum* cultures. Cultures were dark-adapted for 15, prior to measurement. Values were collected using an Imaging Pulse Amplitude Modulated Fluorometer (I-PAM, Walz, Effeltrich, Germany; settings: measuring light = 4, saturation intensity = 8, saturation width = 0.8 s, gain = 3, damping = 3).

Biological replicate	Fv/Fm
1	0.563
2	0.557
3	0.580
4	0.567
5	0.597

Table S2.2: BVOCs detected throughout dataset. All BVOCs (peak normalised to protein content) and their chemical classes that were detected in aposymbiotic anemones, symbiotic anemones and cultures of *B. minutum*. Compounds had to be detected in at least two replicates in at least one symbiotic state. Chemical class was determined based on the molecule's functional group(s). Significance was determined using differential abundance testing and the number of asterisks denotes the size of the adjusted p-value: *<0.05, **<0.01, ***<0.001.

Colour scale *

Zero | Medium | High

BVOC	Aposymbiotic anemones					Symbiotic anemones				Cultured *B. minutum*					Functional Group	Significance
(-)-à-Panasinsen	4.E+03	8.E+03	0	2.E+03	3.E+03	0	0	0	0	0	8E+03	1.E+03	0	0	Sesquiterpene	
1,2,3,4-Tetrahydro-1,8-dimethyl-Naphthalene	4.E+03	1.E+04	3.E+03	5.E+03	7.E+03	0	0	3.E+03	4.E+03	0	3E+03	2.E+02	2.E+03	2.E+02	Aromatic compound	
1,2,3,4-Tetramethylbenzene	3.E+03	8.E+04	4.E+04	6.E+04	3.E+03	3.E+03	3.E+04	1.E+04	4.E+03	0	0	0	0	0	Aromatic compound	*
1,2,3,5,6,7,8,8a-Octahydro-1,8a-dimethyl-7-(1-methylethenyl)-, [1R-(1à,7á,8aà)]-Naphthalene	0	0	0	8.E+03	0	0	0	6.E+03	1.E+04	0	0	0	0	0	Alkene	
1,2,3,5,6,8a-Hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-naphthalene	0	0	0	0	0	0	5.E+03	5.E+03	1.E+04	0	0	0	0	6E+03	Alkene	
1,2,3-Trimethylbenzene	5.E+04	3.E+05	4.E+05	4.E+05	7.E+04	8.E+04	4.E+05	1.E+05	9.E+04	0	0	0	0	0	Aromatic compound	***
1,2,4,5-Tetramethylbenzene	0	5.E+04	2.E+04	3.E+04	3.E+03	0	9.E+03	5.E+03	7.E+03	0	0	0	0	0	Aromatic compound	
1,2-Dibromoethylene	2.E+04	8.E+03	1.E+04	1.E+04	1.E+04	9.E+03	1.E+04	6.E+03	1.E+04	0	0	0	0	0	Halogenated HC	***
1,2-Dichloro-3-methylbenzene	3.E+03	4.E+03	5.E+03	8.E+03	3.E+03	5.E+03	5.E+03	5.E+03	4.E+03	0	0	0	0	0	Halogenated HC	*
1,2-Dichloroethane	5.E+03	3.E+03	6.E+04	5.E+04	1.E+03	5.E+04	5.E+04	4.E+04	0	0	0	0	0	0	Halogenated HC	
1,2-Dihydro-2-methylnaphthalene	0	0	0	0	0	0	0	0	0	0	0	0	2.E+04	9.E+02	Aromatic compound	
1,3-Dichloropropane	5.E+02	0	0	0	0	0	0	0	2.E+02	8.E+03	1.E+04	1.E+04	8.E+03	1.E+04	Halogenated HC	
1,3-Dimethoxybenzene	8.E+03	0	1.E+04	4.E+03	1.E+04	0	0	0	0	4.E+04	2.E+05	2.E+05	6.E+04	2.E+05	Ether	***
1,3-Octadiene	1.E+04	3.E+03	4.E+03	2.E+04	2.E+04	0	3.E+02	0	0	9.E+00	0	0	0	0	Alkene	***
10,18-Bisnorabieta-8,11,13-triene	0	0	0	0	0	0	0	7.E+02	8.E+02	0	0	0	0	0	Aromatic compound	
1-Butanol	0	0	3.E+07	3.E+07	2.E+04	2.E+07	3.E+07	2.E+07	4.E+05	1.E+06	0	2.E+06	3.E+06	0	Alcohol	
1-Ethyl-3-methylbenzene	2.E+05	3.E+05	4.E+05	6.E+05	2.E+05	2.E+05	4.E+05	4.E+05	3.E+05	0	0	0	0	0	Aromatic compound	***
1-Ethyl-4-methylbenzene	2.E+04	7.E+04	7.E+04	1.E+05	3.E+04	3.E+04	7.E+04	8.E+04	6.E+04	0	0	0	0	0	Aromatic compound	***
1-Methyl-1H-pyrrole	8.E+03	4.E+03	4.E+04	4.E+04	3.E+04	1.E+05	2.E+04	1.E+05	9.E+04	3.5E+03	0	3.E+03	2.E+03	2.E+03	DFG	***
1-Pentyl-2-propylcyclopropane	0	0	0	0	0	0	4.E+03	1.E+04	2.E+04	0	0	3.E+03	0	0	Alkane	
1-Pentylheptyl benzene	0	0	7.E+03	0	0	0	7.E+03	0	0	0	0	2.E+04	2.E+04	0	Aromatic compound	
2,3-Butanedione	0	0	0	0	2.E+04	0	1.E+04	3.E+04	0	0	0	0	2.E+05	0	Ketone	
2,4-Dibromo-1-methoxybenzene	7.E+03	7.E+02	7.E+03	9.E+03	1.E+04	5.E+03	4.E+03	1.E+04	9.E+03	8.E+03	3.E+04	4.E+04	1.E+04	4.E+04	DFG	
2,5-Dimethylfuran	8.E+03	2.E+04	6.E+03	9.E+03	1.E+04	5.E+03	1.E+04	3.E+03	1.E+04	2.E+03	1.E+04	1.E+03	1.E+04	1.E+04	Ether	
2,6,11-Trimethyldodecane	0	0	0	0	0	0	0	0	0	0	0	1.E+04	7.E+04	0	Alkane	
2-Bromo-4,6-di-tert-butylphenol	5.E+02	0	4.E+02	4.E+03	3.E+02	4.E+03	3.E+03	1.E+04	1.E+04	0	0	2.E+02	3.E+01	5.E+02	DFG	
2-Butanone	0	0	0	0	0	0	0	0	0	2.E+04	5.E+04	4.E+04	2.E+04	8.E+04	Ketone	***
2-Methyl-2-undecanethiol	0	0	0	0	0	0	0	0	0	0	0	0	1.E+05	1.E+05	Organosulfur	*
2-Methyl-3-hexanone	4.E+02	0	3.E+04	1.E+05	1.E+04	4.E+04	3.E+04	1.E+05	3.E+04	0	0	0	0	0	Ketone	**
2-Methylbutanenitrile	0	1.E+03	0	5.E+03	0	0	0	7.E+03	2.E+04	1.E+04	5.E+04	3.E+04	7.E+04	7.E+04	N-containing compound	*
2-Methylpentanal	0	0	0	0	0	0	0	0	0	1.E+05	1.E+05	2.E+05	2.E+05	3.E+05	Aldehyde	***
2-Pentanone	0	0	0	5.E+04	2.E+04	0	0	9.E+04	5.E+04	5.E+05	5.E+05	6.E+05	8.E+05	1.E+06	Ketone	**
3,3,5-Trimethylcyclohexanone	0	0	0	3.E+03	3.E+03	1.E+05	4.E+04	2.E+03	7.E+03	0	0	0	3.E+03	0	DFG	*
3,3-Dimethyl-2-butanone	0	0	0	1.E+04	2.E+03	0	0	9.E+03	9.E+03	5.E+04	1.E+05	1.E+05	1.E+05	2.E+05	Ketone	**

Table S2.2: continued.

3,4-Dimethyl-2-pentanone	3.E+03	0	2.E+03	1.E+03	2.E+04	0	0	4.E+02	0	1.E+06	3.E+06	2.E+06	2.E+06	5.E+06	Ketone	***
3,5-Dimethyl-2-furyl methyl ketone	0	0	0	4.E+03	3.E+03	0	0	0	0	1.E+04	1.E+04	2.E+04	7.E+04	7.E+04	DFG	***
3,5-Dimethylanisole	0	0	0	0	1.E+03	0	0	0	0	3.E+03	5.E+04	2.E+03	1.E+04	7.E+04	DFG	**
3,5-Dimethyloctane	1.E+04	2.E+04	2.E+04	3.E+04	1.E+04	9.E+03	1.E+04	6.E+02	2.E+04	0	1.E+04	1.E+04	2.E+04	2.E+04	Alkane	
3,7-Dimethylundecane	0	0	9.E+04	1.E+03	6.E+02	8.E+04	4.E+04	1.E+05	8.E+02	0	0	0	0	5.E+03	Alkane	*
3-Ethyl-2,2-dimethyloxirane	0	0	0	0	2.E+02	0	0	8.E+01	5.E+02	4.E+04	5.E+04	5.E+04	9.E+04	1.E+05	Ether	***
3-Methyl-1-butene	8.E+03	0	0	0	0	3.E+04	8.E+03	3.E+04	1.E+04	5.E+04	2.E+04	5.E+04	5.E+04	3.E+04	Alkene	*
3-Methyl-2-butanone	0	0	0	2.E+04	1.E+04	0	0	2.E+01	4.E+03	2.E+06	3.E+06	3.E+06	2.E+06	5.E+06	Ketone	***
3-Methyl-2-pentanone	0	0	0	7.E+03	3.E+03	0	0	2.E+04	1.E+04	8.E+04	1.E+05	1.E+05	2.E+05	3.E+05	Ketone	**
3-Methylheptane	7.E+03	7.E+03	6.E+03	5.E+03	6.E+03	3.E+03	3.E+03	3.E+03	8.E+03	0	4.E+03	0	4.E+03	4.E+03	Alkane	*
3-Methylpentane	3.E+04	3.E+04	3.E+04	2.E+04	2.E+04	2.E+03	3.E+04	2.E+04	3.E+04	0	0	8.E+03	1.E+03	0	Alkane	***
3-Methylundecane	3.E+04	2.E+05	0	1.E+05	1.E+05	7.E+03	1.E+04	0	0	0	0	3.E+04	0	0	Alkane	
3-Pentanone	0	0	0	1.E+05	2.E+04	0	0	1.E+05	9.E+04	0	0	1.E+06	1.E+06	2.E+06	Ketone	
4-(Methylthio)-1-butene	0	0	0	0	0	0	0	0	0	1.E+05	1.E+05	1.E+05	2.E+05	2.E+05	Organosulfur	***
4-Ethyl-1,2-dimethylbenzene	0	8.E+04	2.E+04	5.E+04	6.E+03	0	7.E+03	2.E+04	1.E+04	0	0	0	0	0	Aromatic compound	*
4-Methyl-1-undecene	4.E+04	0	4.E+04	6.E+04	0	3.E+04	2.E+04	6.E+04	6.E+04	0	0	0	0	4.E+03	Alkene	*
4-Methyl-3-hexanone	0	0	0	0	0	0	0	0	0	4.E+04	2.E+04	1.E+05	8.E+04	5.E+04	Ketone	***
Acetic acid	0	0	0	0	0	0	0	0	0	7.E+05	0	3.E+04	6.E+04	0	Carboxylic Acid	*
Acetic acid, butyl ester	0	0	1.E+06	2.E+06	5.E+04	4.E+05	9.E+05	6.E+05	0	0	0	0	0	0	Ester	
Amylene hydrate	5.E+03	0	7.E+03	1.E+04	9.E+03	0	0	0	0	2.E+05	3.E+05	3.E+05	5.E+05	5.E+05	Alcohol	***
a-Neoclovene	1.E+04	1.E+04	2.E+04	4.E+03	1.E+04	1.E+03	0	2.E+03	4.E+03	7.E+02	3.E+03	2.E+03	2.E+03	0	Aromatic compound	*
Anisole	0	0	2.E+03	2.E+03	2.E+03	1.E+03	8.E+02	5.E+03	3.E+03	4.E+03	2.E+04	4.E+04	1.E+04	3.E+04	Ether	*
Bromochloromethane	3.E+04	2.E+04	9.E+03	3.E+04	2.E+04	5.E+04	2.E+04	5.E+04	4.E+04	0	0	0	0	0	Halogenated HC	***
Bromodichloromethane	8.E+05	6.E+05	2.E+06	1.E+06	6.E+05	2.E+06	2.E+06	1.E+06	5.E+05	0	0	0	0	0	Halogenated HC	***
Butanal	0	0	4.E+05	6.E+05	2.E+04	4.E+05	8.E+05	5.E+05	4.E+04	0	0	0	4.E+04	2.E+04	Aldehyde	*
Butyl butyrate	0	0	3.E+07	0	6.E+06	0	2.E+07	0	0	0	0	0	0	0	Ester	
Chloroiodomethane	3.E+03	0	3.E+03	8.E+03	7.E+03	3.E+03	1.E+03	6.E+03	8.E+03	0	0	0	0	0	Halogenated HC	
Cyclohexane	9.E+04	7.E+04	7.E+04	1.E+05	9.E+04	7.E+04	7.E+04	7.E+04	1.E+05	0	0	0	0	1.E+04	Alkane	***
Cyclopentane, methyl-	1.E+05	1.E+05	1.E+05	1.E+05	9.E+04	9.E+04	2.E+04	9.E+04	1.E+05	0	0	0	0	0	Alkane	***
Cyclopentanone	0	0	0	0	1.E+03	0	0	0	0	4.E+04	7.E+04	6.E+04	9.E+04	2.E+05	Ketone	***
Cyclosativene	7.E+03	7.E+04	0	0	4.E+02	0	0	0	0	0	1.E+04	5.E+03	0	0	Alkane	
Decane	0	0	0	0	0	0	0	0	9.E+04	2.E+03	4.E+04	0	0	7.E+04	Alkane	
Dibromochloromethane	3.E+05	2.E+05	7.E+05	6.E+05	2.E+05	6.E+05	6.E+05	3.E+05	2.E+05	0	0	0	0	0	Halogenated HC	***
Dibromomethane	3.E+05	1.E+05	3.E+05	1.E+05	2.E+05	5.E+05	1.E+05	4.E+05	3.E+05	0	0	0	0	0	Halogenated HC	***
Dihydro-(-)-neoclovene-(I)	0	0	0	0	0	0	0	5.E+04	1.E+04	5.E+03	0	1.E+04	1.E+04	0	Alkane	
Diiodomethane	0	0	0	9.E+03	5.E+03	0	0	1.E+04	1.E+04	0	0	0	0	0	Halogenated HC	
Dimethyl sulfide	6.E+04	0	0	3.E+04	3.E+03	5.E+05	5.E+05	3.E+05	8.E+05	9.E+06	9.E+06	8.E+06	5.E+06	1.E+07	Organosulfur	***
Dodecane	0	0	0	0	0	0	2.E+04	5.E+03	3.E+04	0	3.E+04	1.E+04	5.E+03	2.E+04	Alkane	*
Ethyl butyrate	0	0	7.E+04	2.E+05	1.E+04	2.E+04	6.E+04	3.E+04	0	0	0	0	0	0	Ester	
Ethyl ether	0	0	0	0	0	0	0	0	0	4.E+03	1.E+04	4.E+03	2.E+04	1.E+03	Ether	
Ethylcyclopropane	0	0	0	0	0	0	0	0	0	0	7.E+03	0	1.E+04	0	Alkane	
Ethylidenecyclopropane	2.E+04	6.E+03	3.E+04	3.E+04	6.E+03	4.E+05	2.E+05	7.E+05	3.E+05	7.E+05	5.E+05	5.E+05	5.E+05	3.E+05	Alkene	**
Hexadecane	4.E+04	9.E+03	4.E+04	0	0	4.E+04	0	2.E+04	0	0	4.E+03	0	0	0	Alkane	

Table S2.2: continued.

Indane	6.E+03	2.E+04	3.E+04	5.E+04	8.E+03	1.E+04	3.E+04	4.E+04	2.E+04	0	0	0	0	0	Aromatic compound	**
Isobutyl acetate	0	0	2.E+05	4.E+05	4.E+04	5.E+03	1.E+05	9.E+04	0	0	0	0	0	0	Ester	
Isophorone	0	0	0	3.E+03	2.E+03	0	0	0	0	4.E+04	7.E+04	6.E+04	1.E+05	1.E+05	Ketone	***
Isopropylsulfonyl chloride	0	8.E+03	0	1.E+03	0	0	0	2.E+03	1.E+04	1.E+04	7.E+04	5.E+04	9.E+04	1.E+05	DFG	*
Methyl formate	0	1.E+04	2.E+03	2.E+04	5.E+03	0	0	8.E+03	0	0	6.E+03	0	1.E+04	0	Ester	
Methylal	0	0	0	1.E+03	0	0	0	0	0	2.E+04	2.E+05	2.E+04	3.E+04	3.E+04	Ether	***
Methylcyclohexane	7.E+03	2.E+04	6.E+03	3.E+03	5.E+03	4.E+03	5.E+03	0	1.E+04	5.E+02	9.E+03	3.E+03	2.E+03	4.E+03	Alkane	
Nitric acid, butyl ester	0	4.E+03	5.E+04	3.E+04	9.E+02	5.E+04	5.E+04	2.E+04	1.E+03	0	0	0	0	0	DFG	
n-Propyl acetate	0	7.E+02	2.E+04	3.E+04	6.E+03	5.E+03	2.E+04	1.E+04	2.E+04	5.E+03	3.E+03	3.E+03	4.E+03	2.E+03	Ester	
Octylcyclohexane	1.E+02	2.E+03	0	9.E+03	0	9.E+03	0	1.E+04	2.E+04	0	0	0	0	0	Alkane	
Pentamethylbenzene	0	5.E+03	3.E+03	9.E+03	1.E+03	0	6.E+02	8.E+02	9.E+02	0	0	0	0	0	Aromatic compound	
Propylbenzene	5.E+04	8.E+04	1.E+05	1.E+05	4.E+04	5.E+04	9.E+04	7.E+04	5.E+04	0	0	0	0	0	Aromatic compound	***
Styrene	3.E+04	1.E+05	1.E+06	2.E+06	9.E+04	1.E+06	1.E+06	1.E+06	2.E+05	0	0	0	0	0	Aromatic compound	***
Sulfur dioxide	0	0	0	6.E+04	1.E+04	0	0	6.E+04	0	0	0	2.E+04	3.E+04	0	Organosulfur	
Tribromomethane	0	0	5.E+03	1.E+05	8.E+04	0	7.E+04	1.E+05	1.E+05	0	0	0	0	0	Halogenated HC	*
Trichloromethane	1.E+06	9.E+05	2.E+06	1.E+06	7.E+05	1.E+06	1.E+06	1.E+06	7.E+05	0	0	0	0	0	Halogenated HC	***
Tridecane	6.E+04	8.E+04	0	2.E+05	1.E+05	3.E+04	0	0	0	0	0	0	2.E+03	0	Alkane	*
UC(1253, 3.61)	0	0	0	6.E+04	0	0	0	5.E+04	1.E+05	0	0	0	6.E+04	0	Unclassified	
UC(1310, 3.04)	0	0	0	2.E+03	3.E+03	4.E+04	1.E+04	5.E+04	4.E+04	0	0	0	0	0	Unclassified	***
UC(1325, 2.11)	0	0	0	0	0	0	0	0	0	1.E+04	2.E+04	1.E+04	3.E+04	4.E+04	Unclassified	***
UC(1365, 2.24)	2.E+03	0	0	2.E+03	3.E+03	0	0	0	0	2.E+04	4.E+04	2.E+04	3.E+04	8.E+04	Unclassified	***
UC(137, 3.02)	0	3.E+06	0	0	0	1.E+05	0	0	0	2.E+06	0	0	4.E+05	0	Unclassified	
UC(1390, 1.49)	0	0	0	9.E+03	8.E+03	0	0	0	0	0	0	0	8.E+03	0	Unclassified	
UC(1465, 2.63)	1.E+04	0	2.E+03	8.E+03	2.E+04	0	8.E+02	4.E+02	2.E+03	3.E+03	2.E+04	3.E+03	1.E+04	5.E+04	Unclassified	*
UC(1505, 1.60)	3.E+04	9.E+04	3.E+04	0	0	2.E+04	3.E+04	0	0	0	0	0	0	0	Unclassified	
UC(1511.07, 1.91)	0	0	0	0	0	0	0	0	0	0	7.E+04	6.E+04	0	0	Unclassified	*
UC(153.64, 1.13)	0	0	0	0	0	0	0	0	0	0	0	0	8.E+04	4.E+04	Unclassified	*
UC(1530, 1.57)	0	0	0	0	0	0	0	0	0	1.E+04	3.E+04	0	0	0	Unclassified	
UC(1539, 1.56)	0	2.E+05	0	1.E+05	0	5.E+04	0	0	0	0	0	0	5.E+04	0	Unclassified	
UC(1555, 1.61)	3.E+04	0	3.E+04	0	0	2.E+04	0	0	0	0	3.E+04	2.E+04	0	0	Unclassified	
UC(1565, 2.18)	1.E+05	0	3.E+04	9.E+04	2.E+05	0	0	0	0	1.E+05	5.E+05	8.E+04	3.E+05	7.E+05	Unclassified	***
UC(1570, 2.73)	0	0	0	1.E+03	9.E+02	2.E+04	1.E+04	3.E+04	3.E+04	0	0	0	0	0	Unclassified	***
UC(1745, 2.85)	0	0	0	1.E+03	1.E+03	5.E+04	2.E+04	7.E+04	6.E+04	0	0	0	1.E+03	1.E+03	Unclassified	***
UC(1776, 3.18)	0	3.E+02	0	0	0	0	0	0	0	0	7.E+03	2.E+04	0	0	Unclassified	
UC(1794.17, 1.58)	0	0	0	0	0	1.E+03	0	0	2.E+04	0	0	4.E+03	0	0	Unclassified	
UC(1819.44, 1.56)	5.E+02	0	2.E+03	2.E+04	3.E+04	0	6.E+02	1.E+04	0	0	0	6.E+02	2.E+04	4.E+04	Unclassified	
UC(1854.23, 1.588)	0	3.E+03	0	1.E+03	3.E+03	0	0	0	4.E+03	0	0	2.E+02	2.E+02	0	Unclassified	
UC(1888.75, 1.59)	0	0	0	1.E+04	1.E+04	0	0	0	0	0	0	6.E+03	0	9.E+03	Unclassified	
UC(1894.17, 1.75)	0	4.E+04	0	4.E+04	3.E+04	0	0	1.E+04	4.E+03	0	0	0	2.E+04	3.E+03	Unclassified	
UC(1955, 2.18)	0	0	0	4.E+03	2.E+02	0	0	1.E+03	7.E+02	2.E+03	1.E+03	3.E+03	8.E+03	8.E+03	Unclassified	
UC(1962, 1.58)	0	1.E+05	0	3.E+04	0	0	0	0	5.E+04	1.E+04	0	0	0	5.E+04	Unclassified	
UC(1972.33, 1.82)	0	0	0	4.E+04	2.E+04	0	0	3.E+04	3.E+04	4.E+04	4.E+04	3.E+04	0	9.E+04	Unclassified	
UC(1990, 1.49)	0	0	0	0	2.E+04	0	0	0	0	0	0	0	2.E+04	2.E+04	Unclassified	

Table S2.2: continued

UC(2030, 1.59)	0	0	0	1.E+04	0	0	0	1.E+04	5.E+03	0	0	0	9.E+03	0	Unclassified	
UC(2040.83, 1.715)	0	0	3.E+03	4.E+03	0	0	0	4.E+03	0	0	0	0	4.E+03	3.E+03	Unclassified	
UC(2048, 1.57)	0	0	5.E+03	1.E+04	0	0	0	8.E+03	1.E+04	0	0	0	0	9.E+03	Unclassified	
UC(2054.44, 2.25)	0	0	0	8.E+03	4.E+03	0	0	5.E+03	4.E+03	3.E+03	6.E+03	5.E+03	2.E+04	2.E+04	Unclassified	
UC(2055, 2.35)	0	0	0	0	0	0	0	0	0	0	0	0	8.E+03	9.E+03	Unclassified	
UC(2056.25, 2.56)	5.E+03	3.E+03	1.E+03	8.E+03	8.E+03	0	0	7.E+03	7.E+03	4.E+02	1.E+03	5.E+03	0	1.E+03	Unclassified	
UC(2057.22, 1.62)	0	0	8.E+02	5.E+03	0	0	0	0	1.E+04	0	0	0	2.E+04	0	Unclassified	
UC(2059, 1.48)	0	0	0	0	1.E+04	0	0	1.E+04	0	0	0	0	3.E+04	1.E+04	Unclassified	
UC(2115, 1.79)	0	3.E+03	2.E+03	0	0	0	4.E+03	6.E+03	0	2.E+03	0	0	0	0	Unclassified	
UC(2131, 1.58)	0	0	0	0	8.E+03	0	0	0	0	0	1.E+04	0	2.E+04	0	Unclassified	
UC(2138.33, 1.82)	0	0	0	1.E+04	1.E+04	0	0	0	2.E+04	0	1.E+04	0	1.E+04	0	Unclassified	
UC(2141.88, 1.64)	0	0	0	0	0	1.E+03	4.E+03	0	0	9.E+02	0	0	3.E+03	3.E+03	Unclassified	
UC(2146.67, 1.89)	3.E+03	3.E+03	0	0	0	3.E+03	2.E+03	0	0	0	3.E+03	0	0	0	Unclassified	
UC(2188.33, 2.00)	0	0	0	0	1.E+04	0	0	0	0	2.E+04	6.E+04	0	0	0	Unclassified	
UC(2192, 1.91)	0	0	0	0	0	0	0	5.E+03	0	2.E+03	0	6.E+03	9.E+03	0	Unclassified	
UC(220, 1.84)	0	0	1.E+04	0	9.E+03	0	0	0	0	0	0	2.E+04	3.E+04	0	Unclassified	
UC(221.67, 2.07)	0	0	0	7.E+03	2.E+03	7.E+03	5.E+03	2.E+04	2.E+04	0	0	0	0	0	Unclassified	*
UC(2212.78, 1.83)	1.E+04	2.E+04	4.E+03	2.E+04	2.E+04	0	0	1.E+02	0	0	1.E+04	0	7.E+03	3.E+03	Unclassified	***
UC(2267.67, 1.63)	0	1.E+04	4.E+03	0	0	3.E+03	1.E+04	6.E+04	2.E+04	0	0	0	7.E+03	2.E+03	Unclassified	
UC(2280, 1.5)	0	0	0	8.E+04	6.E+04	0	0	0	7.E+04	0	0	0	0	0	Unclassified	
UC(2460, 3.51)	5.E+03	0	9.E+03	2.E+04	4.E+03	0	0	1.E+04	0	1.E+04	3.E+04	8.E+04	4.E+04	6.E+04	Unclassified	**
UC(2570, 2.47)	0	0	2.E+02	2.E+03	0	1.E+04	1.E+04	3.E+04	3.E+04	2.E+03	0	4.E+03	1.E+03	3.E+03	Unclassified	**
UC(267.19, 2.72)	7.E+04	0	2.E+05	6.E+05	3.E+05	0	0	9.E+04	0	0	4.E+06	4.E+06	6.E+06	5.E+06	Unclassified	**
UC(2739.44, 1.87)	0	0	0	3.E+03	0	0	7.E+02	6.E+03	7.E+03	0	0	0	0	0	Unclassified	
UC(362.92, 1.91)	0	0	0	7.E+05	1.E+05	0	0	9.E+05	2.E+06	0	0	0	1.E+06	2.E+05	Unclassified	
UC(385, 2.41)	0	0	0	0	0	0	0	0	0	1.E+05	0	7.E+04	8.E+04	8.E+04	Unclassified	**
UC(415.45, 3.75)	0	0	0	2.E+05	1.E+04	0	0	5.E+05	3.E+06	0	0	0	3.E+04	0	Unclassified	
UC(460.63, 4.19)	2.E+05	2.E+05	2.E+05	0	0	8.E+04	0	0	0	4.E+05	3.E+05	3.E+05	0	0	Unclassified	
UC(483.13, 1.04)	0	0	0	6.E+04	9.E+04	0	1.E+06	0	0	0	0	0	1.E+06	2.E+06	Unclassified	
UC(605, 2.19)	0	3.E+03	3.E+02	3.E+03	2.E+03	1.E+03	1.E+03	4.E+03	5.E+03	2.E+05	6.E+04	7.E+04	6.E+04	9.E+04	Unclassified	*
UC(640, 3.71)	0	0	0	2.E+06	0	0	0	5.E+05	6.E+06	0	0	0	5.E+06	0	Unclassified	
UC(958, 2.55)	0	0	0	7.E+04	0	0	0	2.E+05	2.E+05	0	0	0	2.E+05	0	Unclassified	

Chapter 3

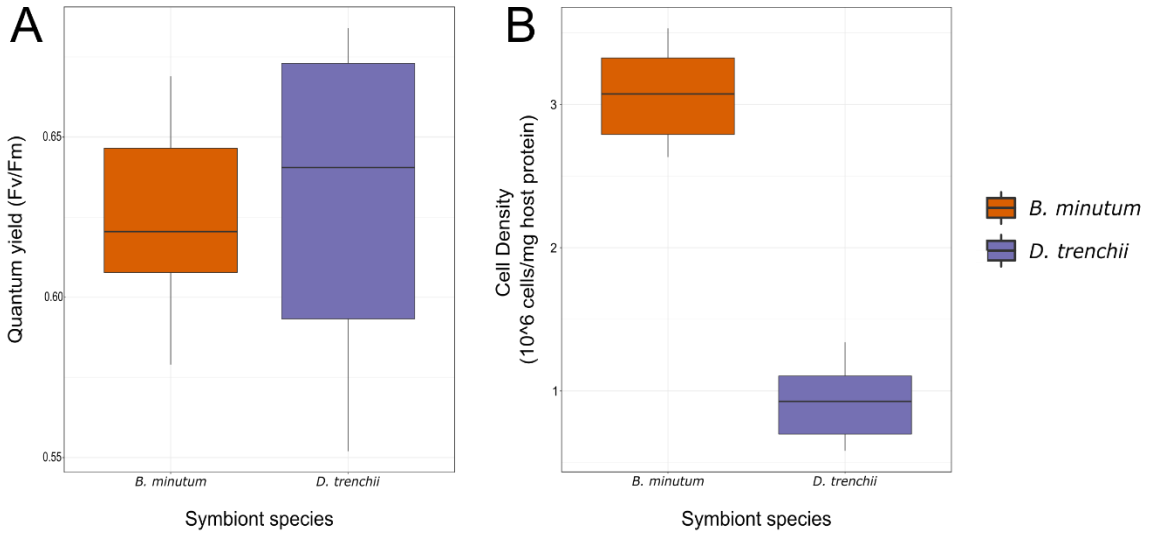

Figure S3.1: A) Maximum photosystem II (PSII) photochemical efficiency (F_v/F_m) and B) symbiont cell densities of holobionts colonised by symbiont species *Breviolum minutum* and *Durusdinium trenchii* taken on day of BVOC and microbial sampling. Whiskers represent minimum and maximum values for this dataset, dots represent individual datapoints. Anemones were dark adapted for 15 min in sampling vials prior to quantum yield measurements.

Table S3.1: Differentially abundant BVOCs (<0.05) detected across 1) aposymbiotic anemones; 2) anemones symbiotic with *D. trenchii* (heterologous) and 3) anemones symbiotic with *B. minutum* (homologous)

BVOC	logFC	AveExpr	P.Value	adj.P.Val	label	Higher_in
1,4-Pentadiene	7.702569	8.170567	5.46E-06	0.000758	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Dimethyl sulphide	7.663887	10.45491	0.000188	0.013084	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Octanal	-6.63861	8.537077	0.001035	0.036232	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Dodecanal	-6.6704	8.357859	0.001043	0.036232	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Nonanal	-7.50741	8.420721	0.001484	0.041256	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
cis-6-Nonenol	-6.28383	7.946443	0.001877	0.043477	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Dimethyl sulphide	9.898329	10.45491	5.14E-07	7.14E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis

1,1,2,2,3,3-Hexamethylindane	-7.68899	6.151933	0.000151	0.010528	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
2-Methoxy-thiazole	6.259711	6.76794	0.000472	0.021864	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
1,4-Pentadiene	-7.43341	8.170567	8.48E-05	0.011789	*B. minutum symbiosis* symbiosis *vs.* *D. trenchii* symbiosis	*B. minutum symbiosis* symbiosis

Table S3.2: Differentially abundant microbes ($p < 0.05$) detected across 1) aposymbiotic anemones; 2) anemones symbiotic with *D. trenchii* (heterologous) and 3) anemones symbiotic with *B. minutum symbiosis* (homologous)

Name	**taxon_ID**	**logFC**	**adj.P.Val**	**label**	**Higher in**
Campylobacteraceae	taxon_2	-11.6377561	1.05E-09	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Vibrionaceae	taxon_20	-9.083924682	3.50E-07	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Bacteroidetes	taxon_35	10.98921978	3.50E-07	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Tepidibacter mesophilus	taxon_33	-8.019097041	4.22E-07	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Gammaproteobacteria	taxon_24	-8.635219055	1.10E-06	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Alphaproteobacteria	taxon_15	-9.14649014	1.10E-06	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Paraglaciecola	taxon_63	8.054035612	6.72E-06	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Proteobacteria	taxon_155	6.774446978	1.02E-05	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Vibrionaceae	taxon_55	-5.933931872	3.38E-05	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Flavobacteriia	taxon_30	-6.89165268	4.99E-05	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Alteromonadaceae	taxon_131	6.698017115	8.15E-05	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis

unclassified	taxon_67	-6.00368853	9.73E-05	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Vibrionaceae	taxon_19	-6.881473481	0.00012738	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Bacteroidetes	taxon_8	-8.38106729	0.00012738	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Rhodobacteraceae	taxon_117	6.344366813	0.000258354	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Polaribacter huanghezhanensis	taxon_62	-5.346774006	0.000258354	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Vibrio sinaloensis	taxon_43	-5.633854016	0.000258354	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Vibrio crosai	taxon_42	-5.38260227	0.00034632	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Bacteroidetes	taxon_29	-6.516638661	0.00034632	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Alteromonadaceae	taxon_95	6.143878047	0.000749625	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
***Chlamydiia* sp.**	taxon_79	6.594860407	0.000756115	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Rhodospirillales	taxon_187	5.115962477	0.001283903	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Flavobacteriales	taxon_146	5.28403114	0.001283903	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
***Labrenzia* sp.**	taxon_161	4.929289156	0.001283903	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
***Chlamydiia* sp.**	taxon_176	4.912479847	0.001283903	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Vibrio crosai	taxon_39	-5.322736099	0.001283903	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Gammaproteobacteria	taxon_143	4.854329288	0.001444656	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
***Parasphingorhabdus* sp.**	taxon_169	4.72459138	0.002352881	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Maritalea porphyrae	taxon_75	-4.857059267	0.002448795	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone

***Cohaesibacter* sp.**	taxon_50	-4.993792627	0.002596865	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Rhodobacteraceae	taxon_17	-4.838214878	0.0029103	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Vibrio crosai	taxon_11	-3.901426652	0.006335499	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Pseudoalteromonas piscicida	taxon_93	-4.11271875	0.006335499	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
***Arcomobacter* sp.**	taxon_18	-5.82323865	0.008380197	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Flavobacteriaceae	taxon_4	-6.858945282	0.009745443	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
***Croceibacter atlanticus* HTCC2559**	taxon_68	-3.715856291	0.012102204	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
unclassified	taxon_38	6.385172422	0.013491098	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Vibrio sinaloensis	taxon_44	-3.926324676	0.017519447	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Proteobacteria	taxon_166	2.993939404	0.022098695	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Rhodobacteraceae	taxon_45	-4.044200152	0.032038917	Aposymbiotic *vs.* *B. minutum* symbiosis	Aposymbiotic anemone
Flavobacteriaceae	taxon_78	3.906151746	0.047384012	Aposymbiotic *vs.* *B. minutum* symbiosis	*B. minutum* symbiosis
Campylobacteraceae	taxon_2	-12.54558197	1.37E-10	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrio crosai	taxon_42	-8.720940695	2.00E-07	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Gammaproteobacteria	taxon_24	-9.543044922	2.29E-07	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrionaceae	taxon_55	-7.697699825	4.13E-07	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Tepidibacter mesophilus	taxon_33	-7.925390564	8.02E-07	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrio sinaloensis	taxon_43	-7.632038079	4.15E-06	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone

Gammaproteobacteria	taxon_61	-7.094961195	9.14E-06	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrio sinaloensis	taxon_44	-7.397723174	2.18E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Bacteroidetes	taxon_8	-9.288893157	3.38E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Polaribacter huanghezhanensis	taxon_62	-6.254599873	3.81E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
unclassified	taxon_67	-6.352450017	4.50E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Flavobacteriia	taxon_30	-6.995921603	4.50E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Cohaesibacter	taxon_50	-7.07681947	4.50E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Bacteroidetes	taxon_29	-7.424464528	6.46E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
***Croceibacter atlanticus* HTCC2559**	taxon_68	-5.927742528	9.47E-05	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrio crosai	taxon_39	-6.412746239	0.000242384	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Alphaproteobacteria	taxon_15	-6.581707156	0.000333199	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Proteobacteria	taxon_166	5.341653404	0.000428386	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Gammaproteobacteria	taxon_128	5.615738594	0.000664363	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Pseudoalteromonas piscicida	taxon_93	-5.020544617	0.001218664	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrio crosai	taxon_11	-4.583049866	0.001537553	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Rhizobiales	taxon_65	5.977279081	0.002575151	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Arcobacter	taxon_18	-6.731064517	0.002718679	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Erythrobacter gaetbuli	taxon_175	4.912908552	0.002765546	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis

Myxococcales	taxon_66	5.415370989	0.007021348	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Cytophagales	taxon_121	4.396457203	0.013454925	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
unclassified	taxon_119	4.634983407	0.013531188	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Flavobacteriaceae	taxon_122	-3.856422311	0.017260377	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Gammaproteobacteria	taxon_174	4.113334599	0.017260377	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Bacteroidetes	taxon_54	-4.217438934	0.017368823	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
***Photobacterium gaetbulicola* Gung47**	taxon_52	-4.217631671	0.018057609	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Oceanospirillaceae	taxon_120	-4.06160099	0.018057609	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Vibrionaceae	taxon_20	-3.385733945	0.020879077	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
***Limimaricola cinnabarinus* LL-001**	taxon_240	3.849855431	0.020879077	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Rhodobacteraceae	taxon_241	3.462514472	0.022291686	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
***Limimaricola* sp.**	taxon_84	3.703038546	0.026208693	Aposymbiotic *vs.* *D. trenchii* symbiosis	*D. trenchii* symbiosis
Vibrionaceae	taxon_19	-3.528020008	0.027453462	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Alphaproteobacteria	taxon_106	-4.091487448	0.030099188	Aposymbiotic *vs.* *D. trenchii* symbiosis	Aposymbiotic anemone
Bacteroidetes	taxon_35	-8.313224035	0.000316696	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Paraglaciecola	taxon_63	-6.907999642	0.000316696	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Proteobacteria	taxon_155	-5.742388621	0.000326894	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis

Rhodobacteraceae	taxon_45	7.045217916	0.000570146	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*D. trenchii* symbiosis
Alteromonadaceae	taxon_95	-6.389639085	0.00116332	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Alteromonadaceae	taxon_131	-5.665958758	0.001373034	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Vibrionaceae	taxon_20	5.698190737	0.001862178	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*D. trenchii* symbiosis
Rhodobacteraceae	taxon_117	-5.312308456	0.004100782	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
***Chlamydiia* sp.**	taxon_79	-5.56280205	0.010863159	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Gammaproteobacteria	taxon_61	-4.225456091	0.022884636	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Rhodospirillales	taxon_187	-4.08390412	0.022884636	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
Rhodobacteraceae	taxon_17	4.325985709	0.022884636	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*D. trenchii* symbiosis
***Labrenzia* sp.**	taxon_161	-3.897230799	0.022884636	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis
***Chlamydiia* sp.**	taxon_176	-3.88042149	0.022884636	*B. minutum* symbiosis *vs. D. trenchii* symbiosis	*B. minutum* symbiosis

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Table S3.3: BVOCs detected throughout dataset. All BVOCs (peak normalised to protein content) and their chemical classes that were detected in aposymbiotic anemones, anemones symbiotic with *B. minutum symbiosis* (homologous symbiosis) and anemones symbiotic with *D. trenchii* (heterologous symbiosis). Compounds had to be detected in at least four replicates in at least one symbiotic state. Chemical class was determined based on the molecule's functional group(s). Significance was determined using differential abundance testing and the number of asterisks denotes the size of the adjusted p-value: *<0.05, **<0.01, ***<0.001.

Colour scale *		
Zero	Medium	High

BVOC	Homologous symbiosis								Heterologous symbiosis								Aposymbiotic anemone								Functional group	Significance
(2,4-cyclopentadien-1-ylidenemethyl)-benzene	4.E+02	0	1.E+03	0	1.E+03	0	2.E+03	0	0	0	4.E+03	0	5.E+03	0	5.E+03	0	0	3.E+02	4.E+03	0	0	0	4.E+03	0	Aromatic compound	
(2-methyl-n-3-propenyl)-(pentamethylcyclopentadienyl)-cobalt	0	3.E+03	0	4.E+03	0	0	0	0	0	2.E+04	0	0	0	1.E+04	0	0	3.E+04	0	0	1.E+04	0	3.E+02	0	3.E+03	Cobalt containing compound	
(E)-Hex-3-enyl (E)-2-methylbut-2-enoate	1.E+02	1.E+02	0	0	2.E+02	0	2.E+02	0	0	0	0	1.E+03	0	0	0	0	0	0	9.E+02	0	0	0	0	0	Ester	
1-(1-propynyl)-cyclohexene	0	2.E+01	0	5.E+01	0	0	0	0	2.E+02	3.E+02	4.E+02	2.E+02	0	1.E+02	2.E+02	1.E+01	0	0	4.E+02	3.E+02	2.E+02	2.E+02	2.E+02	1.E+02	Alkyne	
1-(6-methoxy-2-naphthyl)-ethanol	4.E+01	0	8.E+01	0	5.E+01	0	4.E+01	0	9.E+01	0	9.E+01	0	2.E+02	0	9.E+01	0	0	2.E+02	3.E+02	0	2.E+02	0	8.E+01	0	DFG	
1,1,2,2,3,3-Hexamethylindane	1.E+02	0	0	0	0	0	8.E+01	0	0	0	0	0	0	0	0	0	0	4.E+02	0	1.E+02	3.E+02	1.E+02	3.E+02	5.E+01	Aromatic compound	*
1,1,3-Trimethylindane	2.E+02	0	0	0	0	0	0	0	4.E+02	0	0	0	3.E+02	0	2.E+02	0	0	5.E+02	8.E+02	0	4.E+02	0	3.E+02	0	Aromatic compound	
1,1-dimethyl-1H-indene	3.E+01	0	0	0	0	0	5.E+01	0	0	2.E+02	1.E+02	0	1.E+01	0	9.E+01	0	0	1.E+02	2.E+02	0	4.E+01	0	8.E+01	0	Aromatic compound	
1,2,4-Oxadiazole-3-Methyl-5-pyrid-2-yl	3.E+01	6.E+01	0	0	7.E+01	0	5.E+01	0	0	2.E+02	1.E+02	0	1.E+02	2.E+02	0	0	0	0	2.E+02	6.E+01	0	0	2.E+01	0	DFG	
1,3-Pentanediol, 2,2,4-trimethyl, 1-isobutyrate	0	0	0	0	2.E+01	0	2.E+02	0	1.E+01	2.E+03	2.E+02	0	0	3.E+02	2.E+02	0	3.E+02	3.E+02	0	6.E+02	0	0	0	0	DFG	
1,4-Pentadiene	2.E+02	2.E+02	3.E+02	3.E+02	5.E+02	4.E+02	8.E+02	8.E+02	0	0	0	0	1.E+02	0	3.E+02	3.E+02	0	4.E+02	0	0	0	0	0	0	Alkene	***
10,13-dimethyl-, methyl ester tetradecanoic acid	0	0	7.E+01	0	9.E+01	0	1.E+02	0	0	4.E+02	0	4.E+02	0	0	3.E+02	0	8.E+02	0	3.E+02	0	0	4.E+02	0	4.E+02	Ester	
1-Dimethylamino-2-propyne	0	4.E+02	1.E+02	0	2.E+02	0	2.E+02	0	4.E+02	0	0	0	8.E+02	0	0	0	0	0	2.E+03	0	4.E+02	0	1.E+03	0	Nitrogen containing compound	
1-Methoxy-1-buten-3-yne	2.E+01	0	2.E+01	0	3.E+00	0	6.E+00	0	8.E+01	8.E+01	2.E+02	1.E+01	1.E-01	0	8.E+00	0	1.E+02	2.E+02	2.E+02	0	0	0	0	0	Ether	
1-methyl-1H-Pyrrole	7.E+02	2.E+03	5.E+02	7.E+02	2.E+03	2.E+03	2.E+03	1.E+03	1.E+03	4.E+02	7.E+03	2.E+03	5.E+03	8.E+03	4.E+03	2.E+03	9.E+02	4.E+02	7.E+02	1.E+03	2.E+03	1.E+03	1.E+03	2.E+03	Nitrogen containing compound	
1-Methylethyl-benzene	7.E+02	0	5.E+02	0	2.E+02	0	2.E+02	0	1.E+03	0	1.E+03	0	4.E+02	0	4.E+02	0	3.E+02	3.E+03	4.E+03	0	8.E+02	0	5.E+02	0	Aromatic compound	
1-Methylnapthalene	8.E+02	0	1.E+03	0	1.E+03	0	2.E+03	0	9.E+02	0	8.E+03	0	5.E+03	0	4.E+03	0	0	4.E+03	1.E+04	0	6.E+03	0	4.E+03	0	Aromatic compound	
1-Nitroadamantane	0	0	0	0	0	0	1.E+02	0	0	2.E+02	2.E+02	4.E+02	0	2.E+02	0	0	1.E+02	0	6.E+02	0	2.E+02	7.E+00	0	0	DFG	
2-(1-methylpropyl)-phenol	9.E+02	0	3.E+03	0	0	5.E+01	0	0	0	2.E+03	0	0	0	9.E+02	3.E+03	0	3.E+03	4.E+02	1.E+03	2.E+03	1.E+03	0	0	2.E+03	Alcohol	
2-(4-Formyl-phenoxy)-acetamide	5.E+01	7.E+01	1.E+01	0	6.E-01	0	5.E+02	5.E+01	0	1.E+03	3.E+02	3.E+02	5.E+02	2.E+02	9.E+01	0	1.E+03	2.E+01	2.E+03	1.E+02	4.E+02	2.E+02	0	0	DFG	
2,2-dimethyl-, ethenyl ester pentanoic acid	0	0	7.E+01	1.E+02	6.E+01	0	0	0	6.E+01	0	0	9.E+02	0	4.E+02	0	7.E+00	3.E+02	0	1.E+03	5.E+02	2.E+02	3.E+02	4.E+02	0	Ester	
2,3,3-trimethylcyclobutanone	0	2.E+00	4.E+01	5.E+01	0	0	0	0	2.E+02	0	2.E+02	4.E+02	0	0	0	0	1.E+02	1.E+02	6.E+02	1.E+02	2.E+02	0	0	0	Ketone	
2,3-Butanedione	0	2.E+02	3.E+02	6.E+01	2.E+02	0	0	0	1.E+03	0	1.E+03	0	0	0	0	0	7.E+01	0	3.E+03	0	2.E+02	2.E+02	0	0	Ketone	
2,3-Dihydro-4-methoxyindole-2-one	2.E+02	2.E+02	2.E+02	1.E+02	9.E+01	1.E+02	3.E+02	2.E+02	0	5.E+02	5.E+02	0	4.E+02	6.E+02	3.E+02	8.E+01	0	3.E+02	8.E+02	6.E+02	6.E+02	7.E+02	3.E+02	2.E+02	DFG	
2,5,9-Trimethyldecane	2.E+02	0	0	0	0	4.E+02	6.E+02	1.E+02	0	2.E+03	2.E+03	2.E+03	2.E+03	2.E+03	2.E+03	1.E+02	2.E+03	0	4.E+03	1.E+03	2.E+03	2.E+03	1.E+03	4.E+02	Alkane	
2,6-bis(1,1-dimethylethyl)-4-ethylphenol	0	0	5.E+01	0	2.E+01	4.E+01	1.E+02	3.E+01	0	5.E+02	2.E+02	1.E+02	0	0	2.E+02	0	3.E+02	0	5.E+02	4.E+01	0	0	0	0	Alcohol	
2-Benzylaminoacetonitrile	8.E+00	0	0	0	2.E+02	8.E+01	2.E+02	0	0	3.E+02	8.E+02	8.E+01	6.E+02	2.E+02	5.E+02	2.E+02	2.E+02	0	6.E+02	1.E+02	6.E+02	5.E+02	3.E+02	0	Nitrogen containing compound	
2-bromopropane	0	0	1.E+02	1.E+01	0	0	0	5.E+02	0	0	0	5.E+01	0	0	0	0	0	0	8.E+03	0	3.E+02	8.E+02	2.E+01	0	Halogenated hydrocarbon	
2-Chloro-2,2-difluoro-1-phenylethanone	0	0	0	0	2.E+01	0	3.E+01	3.E+01	0	4.E+02	3.E+02	1.E+03	0	0	2.E+02	0	7.E+02	0	2.E+02	1.E+02	1.E+02	3.E+02	0	0	DFG	
2-Ethyl-1-hexanol	0	0	1.E+03	0	9.E+02	0	0	0	7.E+03	4.E+03	1.E+02	0	0	3.E+02	0	0	1.E+03	1.E+03	3.E+03	0	0	0	0	0	Alcohol	
2-Ethylhexyl hexyl ester sulfurous acid	3.E+02	0	2.E+02	0	7.E+01	1.E+01	4.E+02	0	0	9.E+02	5.E+02	0	8.E+02	0	8.E+02	0	2.E+03	2.E+03	3.E+03	4.E+02	1.E+03	2.E+02	1.E+03	0	Sulphur containing compound	
2-Hydroxyoctyl pentyl sulfoxide	0	0	7.E+01	0	0	5.E+01	0	4.E+01	1.E+02	0	6.E+01	0	2.E+02	0	7.E+01	0	9.E+01	0	6.E+02	1.E+02	1.E+02	1.E+02	0	1.E+02	DFG	
2-Methoxyresorcinol	2.E+02	4.E+02	0	5.E+02	0	3.E+02	0	2.E+02	0	6.E+02	8.E+02	9.E+02	7.E+02	7.E+02	7.E+02	3.E+02	8.E+02	5.E+02	2.E+03	1.E+03	0	1.E+03	0	9.E+02	DFG	
2-Methoxy-thiazole	0	8.E+01	0	0	0	0	4.E+02	5.E+01	0	3.E+02	2.E+02	0	6.E+02	8.E+02	2.E+02	2.E+02	0	0	0	0	0	0	0	0	DFG	*
2-Methyl-1,3,6-Trioxocane	6.E+01	6.E+01	5.E+00	2.E+01	0	0	7.E+01	3.E+01	3.E+01	0	0	0	8.E+01	2.E+02	8.E+00	0	6.E+01	8.E+01	2.E+02	2.E+02	2.E+02	1.E+02	0	0	Ether	

Table S3.3 (cont.):

2-Methyl-1-propene	6.E+01	0	0	0	0	0	0	0	2.E+02	7.E+02	0	3.E+02	0	0	0	1.E+02	3.E+02	0	0	0	0	0	0	1.E+02	Alkene	
2-Methyl-2-phenyl-1,3-benzodioxole	4.E+01	0	1.E+02	0	6.E+01	0	2.E+01	0	2.E+02	6.E+02	8.E+01	4.E+01	0	2.E+01	1.E+02	0	1.E+02	6.E+01	2.E+02	0	6.E+01	2.E+03	0	0	Ether	
2-Methyl-2-propanol	0	0	0	2.E+02	0	0	3.E+02	0	0	0	3.E+02	0	0	0	4.E+01	0	0	0	3.E+03	6.E+02	2.E+02	2.E+03	0	4.E+02	Alcohol	
2-Methylpropyl ester butanoic acid	0	0	0	0	0	0	0	0	1.E+01	0	0	0	0	0	0	0	9.E+02	7.E+02	7.E+02	7.E+02	0	3.E+02	0	0	Ester	
2-Propenal	0	0	0	0	0	0	0	0	5.E+02	4.E+02	0	5.E+02	0	0	6.E+02	0	0	0	1.E+03	0	0	0	0	0	Aldehyde	
3-(3,4-dimethoxyphenyl), (E)-2-propenoic acid	0	1.E+02	2.E+02	0	5.E+01	6.E+00	0	0	0	3.E+02	0	0	3.E+02	2.E+02	3.E+01	0	3.E+02	0	0	0	6.E+02	8.E+02	0	2.E+01	DFG	
3-(4-Methoxyphenyl)-3-methyl-2,5-pyrrolidinedione	0	0	0	0	0	0	4.E+01	6.E+01	0	1.E+02	0	0	0	1.E+02	0	0	0	0	2.E+02	2.E+02	0	2.E+02	9.E+01	0	DFG	
3,3,4-Trimethylheptane	0	6.E+01	0	4.E+02	4.E+02	0	2.E+02	0	9.E+02	1.E+02	0	0	3.E+02	1.E+03	0	0	4.E+02	0	7.E+02	2.E+03	2.E+01	0	0	0	Alkane	
3,3,5-Trimethylcyclohexyl methacrylate	0	0	3.E+03	0	3.E+03	0	4.E+03	0	1.E+03	0	9.E+03	0	1.E+04	0	1.E+04	0	0	0	2.E+04	0	1.E+04	0	1.E+04	0	Ester	
3,3-Dimethylpentane	0	0	0	0	0	0	2.E+02	0	3.E+02	0	0	6.E+02	0	0	8.E+02	3.E+02	8.E+02	0	1.E+03	9.E+02	0	0	7.E+02	0	Alkane	
3,4-Methylenedioxy-N-ethylamphetamine	0	1.E+02	1.E+02	0	0	0	0	0	0	4.E+02	2.E+02	3.E+02	0	0	0	0	2.E+02	0	6.E+02	0	0	0	2.E+02	1.E+02	DFG	
3-Chloro-1H-1,2,4-triazole	0	0	3.E+01	0	0	0	6.E+01	0	0	5.E+02	3.E+02	0	8.E+01	0	0	0	7.E+01	1.E+02	2.E+02	0	2.E+01	2.E+01	0	5.E+01	DFG	
3-Methyl-3-phenyl-azetidine	5.E+01	0	5.E+01	0	4.E-01	0	9.E-01	0	1.E+02	0	1.E+02	0	0	0	0	0	0	4.E+02	3.E+02	0	3.E+01	0	6.E+00	0	Nitrogen containing compound	
3-Methylcyclopentyl acetate	0	1.E+02	0	0	0	0	0	0	0	0	5.E+01	3.E+02	0	0	0	0	1.E+02	0	0	3.E+02	0	1.E+02	1.E+01	0	Ester	
3-Methylnonane	0	0	0	0	8.E+01	0	2.E+02	0	0	0	8.E+02	0	0	0	4.E+02	2.E+02	1.E+03	1.E+03	2.E+03	0	0	0	6.E+02	0	Alkane	
3-Octadecyne	0	2.E+01	4.E+01	0	8.E+01	0	1.E+02	0	0	4.E+02	4.E+02	3.E+02	1.E+02	0	2.E+02	0	5.E+02	0	1.E+03	2.E+02	0	4.E+02	3.E+02	1.E+02	Alkyne	
4-(1,1-dimethylethyl)-benzenepropanal	0	0	0	0	3.E+01	0	2.E+01	0	0	4.E+02	0	3.E+02	0	4.E+02	0	0	8.E+02	0	0	7.E+02	0	5.E+02	0	4.E+02	Aldehyde	
4-(4-butylcyclohexyl)-2,3-dicyano-4-ethoxyphenyl ester benzoic acid	1.E+01	2.E+01	0	0.E+00	1.E+01	0	1.E+01	0	0	0	0	0	0	0	0	0	1.E+02	0	0	0	0	0	0	0	DFG	
4-Ethoxybenzaldehyde	4.E+02	5.E+02	0	4.E+02	0	0	5.E+02	3.E+02	0	0	3.E+02	0	8.E+02	0	8.E+02	8.E+02	2.E+03	0	5.E+02	1.E+03	1.E+03	1.E+03	0	2.E+02	DFG	
4-Hydroxy-2-methylacetophenone	1.E+02	0	0	2.E+01	5.E+01	0	5.E+01	3.E+01	2.E+03	1.E+03	0	1.E+01	3.E+02	1.E+02	6.E+02	2.E+01	7.E+02	1.E+03	0	5.E+02	0	7.E+02	9.E+01	2.E+02	DFG	
5-Methyl-3-isoxazolamine	9.E+01	2.E+02	1.E+02	2.E+02	0	0	0	0	3.E+02	4.E+02	0	4.E+02	0	0	0	0	0	4.E+02	9.E+02	5.E+02	4.E+02	5.E+02	4.E+02	4.E+02	DFG	
6,10-Dimethyl-5,9-undecadien-2-one	0	0	0	0	0	0	0	0	0	0	8.E+02	0	0	0	6.E+02	0	1.E+02	2.E+02	1.E+03	0	2.E+02	5.E+02	0	0	Ketone	
a-amino-, methyl ester benzeneacetic acid	0	2.E+01	0	7.E+00	0	0	7.E+01	4.E+01	0	1.E+02	1.E+02	2.E+02	0	6.E+01	6.E+01	9.E+01	4.E+02	0	6.E+01	0	3.E+02	2.E+02	0	0	DFG	
Acetaldehyde	0	0	2.E+03	0	0	0	0	0	0	0	0	0	0	0	9.E+03	0	0	0	2.E+04	0	2.E+03	7.E+03	7.E+03	0	Aldehyde	
Acetone	0	2.E+02	2.E+03	2.E+03	0	0	4.E+01	0	2.E+03	0	2.E+03	0	0	0	0	0	0	0	3.E+04	0	0	0	0	0	Ketone	
Acetophenone	7.E+01	0	3.E+01	0	4.E+01	0	6.E+01	0	0	1.E+03	9.E+02	2.E+02	0	0	1.E+02	0	2.E+02	6.E+02	1.E+03	1.E+01	0	0	0	0	Ketone	
aR-Himachalene	2.E+02	0	2.E+02	0	1.E+02	0	1.E+02	0	5.E+02	0	5.E+02	0	4.E+02	0	2.E+02	0	0	5.E+02	1.E+03	0	5.E+02	0	2.E+02	0	Aromatic compound	
Benzaldehyde	8.E+01	2.E+02	6.E+01	0	5.E+01	0	2.E+01	0	2.E+02	1.E+03	1.E+03	2.E+02	0	0	0	0	1.E+02	1.E+03	2.E+03	3.E+02	3.E+01	0	0	0	Aldehyde	
Benzene	8.E+01	0	3.E+02	0	3.E+02	0	0	0	6.E+02	6.E+02	5.E+01	0	0	0	0	0	5.E+02	6.E+02	2.E+03	0	2.E+02	0	0	0	Aromatic compound	
Benzophenone	0	0	0	0	0	0	0	0	1.E+01	2.E+04	0	2.E+02	0	3.E+02	0	0	8.E+02	0	0	0	0	0	0	1.E+02	Ketone	
Benzoyl bromide	7.E+02	5.E+02	0	3.E+02	0	4.E+02	0	0	0	0	0	7.E+02	0	0	2.E+03	0	0	0	0	0	0	0	0	0	DFG	
Bicyclo[4.2.0]octa-1,3,5-triene-7,8-dione	0	1.E+02	0	0	0	0	2.E+02	0	0	0	6.E+02	1.E+03	0	3.E+01	1.E+03	0	6.E+02	0	9.E+02	7.E+02	0	0	0	8.E+00	Ketone	
cis-6-Nonenol	0	0	0	0	0	0	8.E+01	0	0	9.E+02	4.E+02	5.E+02	0	0	4.E+02	0	5.E+02	3.E+02	1.E+03	2.E+02	2.E+01	2.E+02	2.E+02	0	Alcohol	*
Cyclohexaneacetic acid	0	0	7.E+01	0	0	0	8.E+01	0	0	5.E+02	3.E+02	8.E+02	0	0	4.E+02	0	6.E+02	0	2.E+03	0	0	6.E+01	6.E+01	2.E+01	Carboxylic acid	
Dec-2-yl 2-fluoroethyl ester glutaric acid	7.E+01	0	0	0	0	0	0	1.E+02	0	2.E+02	3.E+02	0	0	3.E+02	0	0	2.E+02	0	4.E+02	4.E+02	4.E+02	4.E+02	0	0	DFG	
Decane	0	0	0	2.E+02	0	0	2.E+02	5.E+01	2.E+02	1.E+03	7.E+02	8.E+02	0	0	6.E+02	3.E+01	6.E+02	1.E+03	2.E+03	8.E+02	7.E+02	7.E+02	3.E+02	0	Alkane	
Dibromomethane	3.E+02	4.E+02	6.E+02	5.E+02	7.E+02	7.E+02	1.E+03	8.E+02	2.E+02	3.E+02	6.E+02	7.E+02	1.E+03	2.E+03	1.E+03	1.E+03	1.E+02	3.E+01	5.E+02	4.E+02	6.E+02	2.E+02	2.E+03	1.E+03	Halogenated hydrocarbon	
Diethoxymethane	2.E+02	2.E+02	0	3.E+02	2.E+02	0	8.E+02	2.E+02	0	2.E+03	7.E+02	1.E+03	3.E+01	0	4.E+02	0	1.E+02	1.E+03	8.E+03	5.E+02	0	1.E+03	0	0	Ether	
Dimethyl sulphide	1.E+03	1.E+03	2.E+03	9.E+02	1.E+03	1.E+03	0	3.E+02	2.E+03	8.E+02	2.E+03	8.E+02	2.E+03	2.E+03	2.E+03	1.E+03	0	0	0	0	0	0	0	0	Sulphur containing compound	***
Di-tert-butyl peroxide	0	0	0	2.E+03	4.E+03	0	2.E+03	0	8.E+03	0	0	6.E+03	1.E+03	9.E+03	0	0	6.E+03	0	1.E+04	2.E+04	0	0	0	0	Ether	
Docosane	0	1.E+04	8.E+03	0	0	7.E+03	0	4.E+02	0	0	4.E+03	0	6.E+03	4.E+04	0	0	0	0	6.E+04	0	2.E+03	0	1.E+02	0	Alkane	
Dodecanal	0	0	0	0	0	0	2.E+02	0	0	2.E+03	8.E+02	7.E+02	0	0	3.E+02	0	7.E+02	2.E+02	2.E+03	3.E+02	1.E+02	7.E+02	3.E+02	0	Aldehyde	*
Epistephamiersine	5.E+01	7.E+01	3.E+01	0	0	0	0	0	0	5.E+01	2.E+02	2.E+02	0	0	0	0	2.E+02	5.E+01	4.E+02	0	1.E+02	0	0	0	DFG	
Ethylbenzene	2.E+02	0	2.E+02	0	1.E+02	0	2.E+02	0	3.E+02	0	5.E+02	0	4.E+02	0	6.E+02	0	0	4.E+02	1.E+03	0	5.E+02	0	4.E+02	0	Aromatic compound	
Heneicosane	0	2.E+03	0	0	2.E+03	0	4.E+02	0	4.E+03	7.E+03	5.E+03	3.E+03	2.E+03	2.E+03	0	9.E+02	3.E+03	0	8.E+02	0	7.E+03	2.E+03	0	5.E+03	Alkane	

Table 3.3 (cont.):

Heptanal	0	0	0	0	0	0	0	0	0	3.E+02	9.E+01	9.E+02	0	3.E+01	1.E+02	0	3.E+02	3.E+02	9.E+02	0	0	2.E+02	0	0	Aldehyde	
Hexanal	0	0	0	0	0	0	0	0	0	3.E+02	3.E+01	1.E+03	0	0	0	0	7.E+02	7.E+01	1.E+03	0	1.E+02	2.E+02	0	0	Aldehyde	
Homosalate	3.E+02	2.E+02	2.E+01	0	3.E+02	3.E+02	1.E+02	0	0	0	2.E+01	0	1.E+03	0	0	0	7.E+02	3.E+02	0	0	0	0	4.E+02	0	DFG	
Isolongifolene	2.E+03	9.E+01	2.E+03	1.E+02	5.E+02	2.E+02	0	1.E+02	0	9.E+01	3.E+03	5.E+02	2.E+03	7.E+02	0	4.E+02	1.E+02	0	2.E+03	8.E+01	3.E+03	0	0	2.E+02	Alkene	
Isopropyl dodecanoate/ Isopropyl laurate	0	0	7.E+02	0	3.E+02	0	1.E+02	7.E+01	0	4.E+03	4.E+02	2.E+03	0	0	5.E+02	0	1.E+03	0	8.E+02	5.E+02	3.E+02	1.E+03	0	3.E+02	Ester	
Limonene	5.E+01	0	3.E+01	0	0	0	0	0	1.E+02	0	0	5.E+01	0	0	0	0	1.E+02	4.E+02	2.E+02	0	0	5.E+01	1.E+02	0	Alkene	
m-Aminophenyl trifluoromethyl ether	3.E+02	5.E+02	4.E+02	0	0	0	4.E+02	0	0.E+00	9.E+02	0	0	0	1.E+03	9.E+02	0	1.E+03	0	2.E+03	1.E+03	0	1.E+03	1.E+03	1.E+03	DFG	
Mesitylene	2.E+02	3.E+02	1.E+02	1.E+02	0	5.E+00	0	0	5.E+02	5.E+02	4.E+02	4.E+02	3.E+02	5.E+02	4.E+02	0	8.E+02	6.E+02	1.E+03	9.E+02	6.E+02	7.E+02	5.E+02	6.E+02	Aromatic compound	
Methanesulfonyl azide	3.E+02	0	4.E+03	0	2.E+03	0	0	0	8.E+03	1.E+04	4.E+03	1.E+02	1.E+03	0	2.E+03	0	3.E+03	0	4.E+04	0	0	0	0	0	DFG	
Methyl 2,3,5-trichloro-4-methoxybenzoate	0	5.E+01	0	7.E+01	0	2.E+02	0	2.E+02	0	1.E+03	0.E+00	0.E+00	3.E+02	1.E+03	0	2.E+02	0	0	0	0	0	0	0	0	DFG	
Methyl isohexadecanoate	0	1.E+02	3.E+01	0	9.E+01	9.E+00	1.E+02	0	0	1.E+03	2.E+02	2.E+03	2.E+01	5.E+01	5.E+02	0	4.E+03	0	2.E+02	0	1.E+02	1.E+02	0	5.E+02	Ester	
Methyltriglycol acetate	4.E+01	0	0	0	0	0	3.E+01	2.E+01	0	6.E+01	8.E+01	5.E+01	0	7.E+01	3.E+00	0	4.E+01	6.E+01	1.E+02	1.E+02	1.E+02	0	0	0	DFG	
N-(4-Methoxybenzyl)-1,3-thiazol-2-amine	3.E+01	5.E+01	0	0	0	2.E+01	6.E+01	4.E+01	0	2.E+02	0	0	0	0	0	0	1.E+02	8.E+01	0	9.E+01	0	0	0	0	DFG	
N,3-dimethyl-N-(2-phenylethyl)-benzeneethanamine	5.E+02	0	1.E+02	0	2.E+02	0	2.E+02	0	2.E+03	0	7.E+02	0.E+00	5.E+02	0	6.E+02	0	0	2.E+03	4.E+03	0	1.E+03	0	4.E+02	0	Nitrogen containing compound	
N,N-Dimethyl-3-butoxypropylamine	2.E+01	0	0	0	0	4.E+02	0	2.E+02	0	2.E+03	0	5.E+02	0	1.E+03	1.E+03	0	8.E+02	2.E+03	2.E+03	2.E+02	0	9.E+02	9.E+02	1.E+03	DFG	
Naphthalene	5.E+02	0	5.E+02	0	3.E+02	0	3.E+02	0	8.E+02	0	2.E+03	0	9.E+02	0	9.E+02	0	0	2.E+03	3.E+03	0	1.E+03	0	8.E+02	0	Aromatic compound	
Nonanal	0	0	0	0	0	0	0	0	0	4.E+03	3.E+03	1.E+04	0	1.E+02	0	0	2.E+03	3.E+03	1.E+04	1.E+03	0	5.E+02	2.E+03	0	Aldehyde	*
Nonanoic acid	7.E+02	4.E+02	0	0	0	0	2.E+03	0	0	2.E+03	6.E+03	2.E+04	0	4.E+02	1.E+04	1.E+03	1.E+04	7.E+02	0	2.E+03	4.E+03	5.E+03	0	7.E+03	Carboxylic acid	
N-phenylethanethioamide	9.E+01	0	1.E+02	0	9.E+01	0	9.E+01	0	0	0	2.E+02	0	0	0	2.E+02	0	0	0	0	0	0	0	0	0	DFG	
Octanal	0	0	0	0	6.E+01	0	0	0	0	9.E+02	5.E+02	4.E+03	0	4.E+00	2.E+02	0	1.E+03	6.E+02	4.E+03	2.E+02	1.E+02	9.E+02	3.E+02	0	Aldehyde	*
o-cyclopropanecarbonyl-o-'isobutyryl-1,2-benzenediol	4.E+01	3.E+01	7.E+01	0	8.E+01	0	3.E+01	0	1.E+02	0	0	3.E+01	1.E+02	0	1.E+02	0	2.E+02	1.E+02	4.E+02	2.E+01	2.E+02	1.E+02	0	1.E+01	Ester	
Phenol	1.E+02	0	0	4.E+01	0	0	2.E+02	0	0	1.E+03	5.E+02	3.E+02	2.E+02	2.E+02	3.E+02	0	4.E+02	1.E+03	4.E+02	2.E+02	0	0	2.E+01	0	Alcohol	
Phenyl buta-2,3-dienyl ether	2.E+01	0	0	0	9.E+00	0	2.E+01	0	9.E+01	0	7.E+01	0	0	0	3.E+01	0	0	2.E+02	2.E+02	0	5.E+01	0	7.E+01	0	Ether	
p-Toluic acid, tridec-2-ynyl ester	0	0	3.E+02	0	2.E+02	4.E+02	1.E+02	0	6.E+02	4.E+03	4.E+02	0	0	0	5.E+02	0	0	7.E+01	8.E+02	2.E+02	2.E+03	2.E+03	0	0	DFG	
p-Xylene	9.E+02	0	1.E+03	0	5.E+02	0	9.E+02	0	2.E+03	0	2.E+03	0	3.E+03	0	2.E+03	0	0	2.E+03	4.E+03	0	3.E+03	0	2.E+03	0	Aromatic compound	
Styrene	3.E+02	2.E+02	3.E+02	1.E+02	2.E+02	2.E+01	1.E+02	7.E+01	9.E+02	5.E+02	9.E+02	5.E+02	5.E+02	3.E+02	7.E+02	0	5.E+02	9.E+02	2.E+03	5.E+02	8.E+02	6.E+02	8.E+02	3.E+02	Aromatic compound	
Tert-butyl ester salicylic acid	0	0	3.E+02	0	0	0	0	0	0	1.E+02	8.E+02	6.E+02	0	0	1.E+03	0	1.E+04	0	3.E+01	0	1.E+02	0	0	2.E+03	DFG	
Tetrachloroethylene	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5.E+01	0	0	0	0	4.E+01	5.E+01	7.E+01	Halogenated hydrocarbon	
Tetradecane	0	0	1.E+03	0	0	0	0	1.E+02	0	3.E+03	0	4.E+03	0	8.E+02	0	7.E+01	4.E+03	1.E+03	0	1.E+03	0	2.E+03	0	9.E+02	Alkane	
Toluene	1.E+03	0	1.E+03	0	6.E+02	0	8.E+02	0	3.E+03	0	3.E+03	0	4.E+03	0	2.E+03	0	0	3.E+03	7.E+03	0	5.E+03	0	1.E+03	0	Aromatic compound	
trans-1,4-Cyclohexanediol, bis(heptafluorobutyrate)	0	0	0	0	0	2.E+02	0	0	0	0	0	1.E+02	2.E+02	0	2.E+02	1.E+02	0	0	0	0	0	3.E+02	2.E+02	3.E+02	DFG	
UC(14.243)	0	2.E+02	0	7.E+01	0	8.E+01	0	5.E+01	0	2.E+02	0	2.E+02	0	2.E+02	0	5.E+01	7.E+02	0	0	3.E+02	0	3.E+02	0	1.E+02	Unclassified	
UC(14.82)	1.E+02	9.E+01	4.E+01	9.E+01	0	2.E+01	2.E+02	2.E+01	0	5.E+02	2.E+02	2.E+02	2.E+02	2.E+02	3.E+01	0	6.E+01	4.E+02	6.E+02	1.E+02	4.E+02	2.E+02	0	2.E+01	Unclassified	
UC(19.747)	5.E+01	1.E+02	5.E+01	0	0	0	8.E+01	6.E+01	1.E+02	1.E+02	2.E+02	1.E+02	4.E+02	5.E+02	0	0	3.E+02	1.E+02	9.E+02	5.E+02	4.E+02	3.E+02	5.E+01	0	Unclassified	
UC(27.28)	5.E+01	1.E+02	6.E+01	5.E+01	0	3.E+01	2.E+00	4.E+00	2.E+02	2.E+02	1.E+02	3.E+02	2.E+02	2.E+02	1.E+02	0	3.E+02	0.E+00	5.E+02	4.E+02	3.E+02	0	2.E+02	3.E+02	Unclassified	
UC(27.756)	5.E+01	2.E+02	0	0	2.E+02	1.E+02	3.E+01	4.E+01	0	5.E+02	3.E+02	7.E+02	6.E+01	4.E+01	4.E+02	4.E+01	5.E+02	0	0	8.E-01	0	0	4.E+01	0	Unclassified	
UC(33.81)	1.E+02	0	0	0	4.E+02	9.E+01	3.E+02	1.E+02	0	1.E+03	0	0	2.E+02	8.E+02	1.E+02	1.E+02	0	0	0	0	0	0	1.E+02	0	Unclassified	
UC(35.86)	0	6.E+01	0	0	0	0	3.E+02	0	0	3.E+02	8.E+02	3.E+03	0	2.E+02	2.E+03	0	2.E+03	6.E+01	0	0	0	5.E+02	0	7.E+02	Unclassified	
UC(36.84)	5.E+02	0	4.E+02	0	2.E+02	0	2.E+02	0	1.E+03	0	1.E+03	0	8.E+02	0	3.E+02	0	0	2.E+03	3.E+03	0	1.E+03	0	6.E+02	0	Unclassified	
UC(37.94)	5.E+01	0	0	0	0	0	3.E+01	2.E+01	0	2.E+02	8.E+01	7.E+01	0	8.E+01	1.E+02	0	4.E+01	0	5.E+02	2.E+02	0	9.E+01	1.E+02	6.E+01	Unclassified	
UC(39.23)	0	0	0	0	0	0	0	0	0	9.E+02	4.E+02	1.E+02	0	2.E+02	3.E+02	0	2.E+02	0	6.E+02	0	0	0	3.E+02	0	Unclassified	
UC(41.47)	7.E+01	0	6.E+01	0	0	0	0	0	0	0	2.E+02	0	1.E+02	0	1.E+02	0	0	3.E+02	4.E+02	0	2.E+02	0	1.E+02	0	Unclassified	
UC(41.51)	0	0	0	0	0	0	8.E+01	0	0	0	2.E+02	3.E+02	0	0	1.E+02	0	2.E+02	0	4.E+02	0	2.E+02	0	2.E+02	0	Unclassified	
UC(42.08)	0	0	6.E+01	0	0	0	0	0	4.E+02	0	9.E+02	0	3.E+02	0	2.E+01	0	0	9.E+02	1.E+03	0	2.E+02	0	5.E+00	0	Unclassified	
UC(42.13)	9.E+01	0	0	0	0	0	9.E+01	0	2.E+02	0	3.E+02	0	3.E+02	0	2.E+02	0	0	0	5.E+02	0	0	0	2.E+02	0	Unclassified	

Table S3.3 (cont.):

UC(42.15)	0	3.E+01	2.E+02	0	2.E+02	0	2.E+01	0	4.E+01	1.E+03	0	1.E+01	0	7.E+01	9.E+00	0	9.E+01	0	5.E+02	1.E+01	0	0	3.E+01	0	Unclassified	
UC(42.61)	2.E+02	0	1.E+02	0	0	0	9.E+01	0	0	0	4.E+02	0	3.E+02	0	2.E+02	0	0	6.E+02	7.E+02	0	3.E+02	0	2.E+02	0	Unclassified	
UC(43.02)	0	6.E+01	0	7.E+01	0	5.E+01	0	7.E+01	0	1.E+02	0	1.E+02	0	2.E+02	0	4.E+01	2.E+02	9.E+01	0	3.E+02	0	1.E+02	0	3.E+02	Unclassified	
UC(43.09)	0	0	0	0	0	1.E+02	0	0	0	4.E+02	0	2.E+02	0	2.E+02	0	0	3.E+02	0	0	3.E+02	0	3.E+02	0	3.E+02	Unclassified	
UC(43.62)	9.E+01	9.E+01	0	5.E+01	0	6.E+01	9.E+01	5.E+01	0	0	3.E+02	2.E+02	0	2.E+02	2.E+02	1.E+02	3.E+02	0	0	3.E+02	3.E+02	0	2.E+02	2.E+02	Unclassified	
UC(44.31)	0	0	0	0	7.E+00	3.E+01	2.E+01	9.E-01	0	0	0	0	0	3.E+01	0	3.E+00	0	0	8.E+01	6.E+00	0	0	1.E+00	0	Unclassified	
UC(44.35)	6.E-01	1.E+02	1.E+02	0	8.E+01	0	4.E+01	0	2.E+02	6.E+02	4.E+01	0	2.E+02	0	2.E+02	0	3.E+03	1.E+03	3.E+02	1.E+02	3.E+02	5.E+01	4.E+02	0	Unclassified	
UC(44.37)	1.E+00	4.E+01	7.E+01	0	0	0	4.E+01	2.E+01	0	2.E+02	2.E+02	3.E+02	0	1.E+02	3.E+02	0	5.E+02	4.E+01	4.E+02	6.E+00	2.E+02	2.E+02	0	0	Unclassified	
UC(44.45)	0	0	3.E+01	0	9.E+01	0	4.E+01	0	0	2.E+02	0	4.E+01	6.E+01	2.E+00	1.E+02	0	0	0	0	8.E+00	9.E+01	0	0	3.E-01	Unclassified	
UC(44.59)	0	7.E+01	0	0	2.E+02	0	9.E+02	0	1.E+02	4.E+02	5.E+02	0	0	5.E+02	0	0	0	3.E+02	7.E+02	3.E+02	4.E+02	7.E+02	0	0	Unclassified	
UC(45.46)	1.E+02	2.E+02	0	0	0	0	2.E+02	0	0	5.E+02	0	4.E+02	0	0	3.E+02	0	5.E+02	3.E+02	7.E+02	4.E+02	0	6.E+02	4.E+02	0	Unclassified	
UC(45.55)	9.E+01	8.E+01	0	0	2.E+01	0	3.E+01	0	0	0	0	2.E+02	0	0	0	0	0	2.E+02	0	0	1.E+02	0	0	0	Unclassified	
UC(45.60)	4.E+01	2.E+01	0	0	3.E+01	0	0	0	1.E+02	0	2.E+02	0	1.E+02	0	2.E+02	0	0	2.E+02	3.E+02	2.E+02	1.E+02	0	1.E+02	0	Unclassified	
UC(45.67)	0	0	2.E+02	0	1.E+02	0	9.E+00	0	0	2.E+03	1.E+02	5.E+02	0	9.E+00	9.E+01	0	9.E+02	0	4.E+02	1.E+02	0	2.E+02	0	0	Unclassified	
UC(46.40)	1.E+01	0	1.E+02	0	4.E+01	2.E+01	8.E+01	0	0	5.E+02	4.E+02	1.E+02	2.E+01	0	1.E+02	0	0	0	3.E+02	0	2.E+02	2.E+02	0	0	Unclassified	
UC(47.66)	0	1.E+02	0	4.E+01	0	0	0	3.E+01	3.E+03	4.E+03	0	0	0	2.E+02	0	9.E+01	0	9.E+02	2.E+02	4.E+02	0	0	0	0	Unclassified	
Z-4-Dodecenol	0	0	0	0	0	0	2.E+02	0	0	2.E+03	1.E+03	2.E+03	0	0	1.E+03	0	1.E+03	5.E+02	2.E+03	5.E+02	0	5.E+02	8.E+02	0	Alcohol	

Table S3.4: Bacterial taxa (ASV counts) detected throughout dataset. All bacteria that were detected in aposymbiotic anemones, anemones symbiotic with *B. minutum symbiosis* (homologous symbiosis) and anemones symbiotic with *D. trenchii* (heterologous symbiosis). Bacteria had to be detected in at least three replicates in at least one symbiotic state to be included. Significance was determined using differential abundance testing and the number of asterisks denotes the size of the adjusted p-value: *<0.05, **<0.01, ***<0.001.

Name	Taxon ID	Aposymbiotic anemone					Heterologous symbiosis					Homologous symbiosis					Significance
Aestuariibacter halophilus	taxon_60	98	0	256	58	0	37	115	90	103	48	103	0	117	32	0	
Alphaproteobacteria	taxon_15	3744	929	1706	4441	1243	0	49	706	0	11	0	18	0	0	0	
Alphaproteobacteria	taxon_106	146	0	7	26	84	0	0	0	0	0	0	0	0	0	12	*
Alphaproteobacteria	taxon_111	95	0	2	58	0	13	30	8	0	43	0	0	0	0	0	*
Alphaproteobacteria	taxon_113	62	0	17	162	0	0	0	0	0	0	0	0	0	0	0	*
Alphaproteobacteria	taxon_115	0	5	9	99	23	4	3	27	20	3	0	18	16	0	0	
Alphaproteobacteria	taxon_140	13	0	0	14	0	0	3	57	0	48	0	0	0	0	0	
Alphaproteobacteria	taxon_173	12	0	0	22	18	0	0	21	0	0	0	7	0	0	0	
Alphaproteobacteria	taxon_184	34	0	12	17	0	0	0	0	0	0	0	0	0	0	0	
Alphaproteobacteria	taxon_194	19	4	0	0	4	2	0	0	15	0	0	0	15	0	0	
Alphaproteobacteria	taxon_261	0	0	0	0	0	0	7	5	14	0	4	0	0	0	0	
Alphaproteobacteria	taxon_318	6	0	4	10	0	0	0	0	0	0	0	0	0	0	0	
Alteromonadaceae	taxon_64	153	17	67	141	19	61	111	143	104	56	49	0	20	25	0	
Alteromonadaceae	taxon_95	0	0	0	0	14	0	0	0	0	0	103	206	13	40	0	**
Alteromonadaceae	taxon_131	0	0	0	0	0	0	0	0	0	0	31	22	37	0	72	***
Alteromonas sp.	taxon_49	229	36	121	344	39	52	68	65	151	169	244	131	96	77	43	
Alteromonas sp.	taxon_71	110	0	84	110	36	0	45	0	27	36	107	0	70	47	0	
Alteromonas simiduii	taxon_85	64	0	61	112	0	0	40	23	21	54	56	16	26	0	8	
Arcobacter sp.	taxon_18	5479	150	2619	9	0	0	0	0	0	0	0	0	0	0	0	**
Bacteroidetes	taxon_8	17054	0	1466	1640	853	0	0	0	0	0	0	0	0	0	0	***
Bacteroidetes	taxon_29	3623	0	303	287	254	0	0	0	0	0	0	0	0	0	0	***
Bacteroidetes	taxon_35	0	0	0	0	0	29	0	0	0	0	25	1054	1113	516	186	***
Bacteroidetes	taxon_54	93	36	503	525	53	3	35	0	11	0	23	12	26	0	9	*
Bacteroidetes	taxon_235	29	0	3	5	0	0	0	0	0	0	0	0	0	0	0	
Bacteroidetes	taxon_247	12	0	0	14	8	0	0	0	0	0	0	0	0	0	0	
Balneola alkaliphila	taxon_262	5	0	16	8	0	0	0	0	0	0	0	0	0	0	0	
Betaproteobacteria	taxon_170	27	0	9	47	0	0	0	0	0	0	0	0	0	0	0	
Campylobacteraceae	taxon_2	6535	5882	1892	20835	5691	0	0	0	0	0	0	0	0	0	0	***
Chlamydiia sp.	taxon_79	0	0	0	0	0	0	0	0	0	0	25	359	0	0	149	**
Chlamydiia sp.	taxon_150	0	26	61	14	0	0	0	0	0	0	0	0	0	11	0	
Chlamydiia sp.	taxon_176	0	0	0	0	0	0	0	0	0	0	0	27	45	0	3	**
Cohaesibacter sp.	taxon_50	1398	19	68	300	58	0	0	0	0	0	0	0	0	0	10	***
Croceibacter atlanticus	taxon_68	603	7	86	127	9	0	0	0	0	0	3	0	7	0	0	***
Crocinitomicaceae	taxon_1	6255	21	2012	17302	777	341	2582	2088	6778	5158	395	156	266	221	346	
Cutibacterium acnes	taxon_167	13	2	0	0	0	0	0	42	0	11	5	0	0	4	5	
Cytophagales	taxon_121	0	0	0	0	0	0	3	0	186	24	0	0	0	0	0	*
Devosia subaequoris	taxon_236	0	2	11	0	18	0	0	0	0	6	0	0	0	0	0	
Donghicola eburneus	taxon_57	276	39	65	236	22	0	18	41	318	171	0	97	0	0	6	*
Ekhidna lutea	taxon_179	0	0	0	21	0	4	9	0	0	0	9	17	0	0	10	

Table (S3.4 cont.):

Erythrobacter gaetbuli	taxon_175	0	0	0	0	0	5	10	16	0	45	0	0	0	0	0	
Flavobacteriaceae	taxon_4	16491	299	5693	2526	0	22	29	127	305	402	0	0	161	0	0	*
Flavobacteriaceae	taxon_22	3729	0	322	365	135	24	147	258	445	767	15	682	114	0	198	
Flavobacteriaceae	taxon_36	168	20	97	15	0	0	0	578	0	432	350	1091	0	146	21	
Flavobacteriaceae	taxon_69	279	5	125	129	22	11	38	10	7	19	9	0	102	26	15	
Flavobacteriaceae	taxon_76	513	0	46	6	0	0	0	0	0	0	0	0	0	0	0	*
Flavobacteriaceae	taxon_78	0	0	6	0	0	0	3	62	180	0	0	277	30	0	0	
Flavobacteriaceae	taxon_87	339	0	39	38	10	0	9	0	0	16	0	0	0	5	7	
Flavobacteriaceae	taxon_122	102	10	53	18	0	0	0	0	0	0	0	14	0	0	0	**
Flavobacteriaceae	taxon_135	33	0	42	21	0	0	0	24	0	8	0	0	25	0	0	
Flavobacteriaceae	taxon_165	36	6	0	0	33	0	0	0	0	14	0	0	0	0	0	
Flavobacteriales	taxon_74	31	10	180	49	86	8	46	0	8	0	7	0	150	0	17	
Flavobacteriales	taxon_146	0	0	0	0	0	0	4	0	0	0	7	61	52	0	0	*
Flavobacteriia	taxon_30	3276	31	878	199	17	0	0	0	0	6	0	0	0	0	0	**
Gammaproteobacteria	taxon_9	2120	596	1707	3438	2339	460	990	1365	203	719	735	2172	1209	46	156	
Gammaproteobacteria	taxon_21	1035	358	998	1078	1094	90	0	546	332	124	231	1133	369	35	125	
Gammaproteobacteria	taxon_24	1510	1180	98	690	3452	0	0	0	0	0	0	0	0	0	0	***
Gammaproteobacteria	taxon_25	691	303	826	870	736	40	17	462	337	103	176	860	313	39	146	
Gammaproteobacteria	taxon_26	234	173	1130	652	463	101	8	38	2028	248	237	304	74	112	17	
Gammaproteobacteria	taxon_47	180	44	150	52	98	12	43	766	194	179	38	180	26	48	0	
Gammaproteobacteria	taxon_61	255	31	419	158	86	0	0	0	0	0	0	11	62	0	15	***
Gammaproteobacteria	taxon_102	11	0	0	0	35	0	10	21	12	45	17	136	19	0	0	
Gammaproteobacteria	taxon_126	0	20	0	46	117	0	0	0	0	0	0	0	0	0	0	*
Gammaproteobacteria	taxon_128	0	0	0	0	0	0	23	5	126	29	0	0	0	0	0	***
Gammaproteobacteria	taxon_143	0	0	0	0	0	0	0	0	8	0	6	111	9	0	0	*
Gammaproteobacteria	taxon_174	0	0	0	0	5	6	0	29	31	8	0	0	0	0	0	
Hyphomonadaceae	taxon_109	76	0	43	4	16	15	11	12	22	12	0	0	9	34	4	
Hyphomonas sp.	taxon_103	42	11	26	14	77	0	19	64	8	33	0	0	0	8	3	*
Labrenzia sp.	taxon_161	0	0	0	0	0	0	0	0	0	0	0	80	11	0	4	**
Leeuwenhoekiella aequorea	taxon_53	377	46	229	194	94	32	11	62	26	48	43	87	61	98	0	
Limimaricola sp.	taxon_84	32	0	4	35	4	34	10	128	57	42	7	14	97	0	19	
Limimaricola cinnabarinus	taxon_240	0	0	0	0	0	12	0	14	5	0	5	0	0	0	0	
Maricaulis maris	taxon_46	411	60	280	144	201	24	133	185	220	133	17	41	79	91	4	
Marinilabiliales	taxon_99	204	0	0	18	130	0	0	0	0	0	0	0	0	0	0	*
Marinobacter salarius	taxon_89	74	8	110	65	36	9	0	29	39	29	9	24	9	13	5	
Marinoscillum sp.	taxon_198	0	0	14	15	0	0	4	0	12	8	0	0	0	5	0	
Maritalea sp.	taxon_107	0	0	23	48	57	0	0	0	0	20	17	37	67	0	0	
Maritalea porphyrae	taxon_56	292	30	49	157	245	41	40	32	10	0	119	156	89	25	11	
Maritalea porphyrae	taxon_75	106	161	27	80	27	0	21	101	0	50	0	0	0	0	0	***
Myxococcales	taxon_66	31	0	0	0	0	0	30	64	56	59	0	617	0	0	0	*
Oceanospirillaceae	taxon_51	488	0	339	0	0	0	0	364	0	0	51	0	330	56	8	
Oceanospirillaceae	taxon_120	87	24	0	25	80	0	0	0	0	0	0	0	0	0	0	**

Table S3.4 (cont.):

Oceanospirillales	taxon_130	0	6	41	12	91	0	3	0	0	0	0	0	19	0	0	
Oligoflexia	taxon_230	9	0	0	23	6	0	0	0	0	0	0	0	0	0	0	
Owenweeksia sp.	taxon_27	1702	105	1655	284	157	38	36	95	182	137	17	471	117	21	7	
Paraglaciecola sp.	taxon_63	0	0	0	9	0	0	0	20	0	0	27	267	611	29	7	***
Parasphingorhabdus sp.	taxon_169	0	0	0	0	0	0	0	0	0	9	0	61	10	5	0	*
Photobacterium gaetbulicola	taxon_40	202	100	693	340	138	0	70	317	167	55	116	406	80	79	0	
Photobacterium gaetbulicola	taxon_52	217	42	337	214	89	0	0	156	53	0	48	240	34	0	6	*
Photobacterium gaetbulicola	taxon_88	35	0	135	64	29	0	0	100	27	0	0	73	0	0	0	
Phyllobacteriaceae	taxon_77	193	27	78	79	0	0	0	0	37	91	0	0	39	18	0	
Pleionea mediterranea	taxon_136	44	3	4	0	20	3	20	34	8	5	0	0	9	0	0	
Polaribacter huanghezhanensis	taxon_62	778	8	106	125	17	0	0	0	0	0	0	0	0	0	0	***
Proteobacteria	taxon_94	87	26	69	0	80	28	11	24	0	55	0	0	0	0	0	*
Proteobacteria	taxon_114	0	0	26	158	0	0	0	8	17	0	0	0	12	13	4	
Proteobacteria	taxon_152	13	0	14	13	31	0	0	37	0	0	0	0	0	0	0	
Proteobacteria	taxon_155	0	0	0	0	0	0	0	0	0	0	7	52	26	6	14	***
Proteobacteria	taxon_166	0	0	0	0	0	5	5	16	12	15	0	36	0	0	0	
Pseudoalteromonas sp.	taxon_92	66	16	65	47	26	0	9	22	46	0	0	48	34	20	0	
Pseudoalteromonas arabiensis	taxon_37	595	114	491	293	244	17	21	240	196	88	107	283	133	48	16	
Pseudoalteromonas piscicida	taxon_93	180	0	90	96	19	0	0	0	0	0	0	0	0	0	0	***
Pseudoteredinibacter isoporae	taxon_112	112	0	6	108	0	0	0	0	0	0	10	0	7	0	0	
Rhizobiales	taxon_65	0	0	0	0	9	3	5	6	398	409	0	101	0	0	0	**
Rhizobiales	taxon_96	104	0	16	18	29	0	0	61	0	58	6	77	0	4	0	
Rhizobiales	taxon_202	0	0	27	17	10	0	0	0	0	0	0	0	0	0	0	
Rhizobium subbaraonis	taxon_41	962	70	297	193	95	50	66	147	39	291	51	80	140	35	69	
Rhodobacteraceae	taxon_17	2540	285	503	2494	1668	36	494	518	1232	512	0	66	106	66	0	*
Rhodobacteraceae	taxon_23	850	68	355	646	84	170	220	1221	534	981	194	875	755	64	50	
Rhodobacteraceae	taxon_45	905	9	0	138	47	33	63	72	429	401	0	0	0	0	0	***
Rhodobacteraceae	taxon_104	231	0	0	16	48	0	0	0	0	0	0	0	0	0	0	*
Rhodobacteraceae	taxon_117	0	0	0	0	0	0	0	0	0	0	0	148	8	63	3	***
Rhodobacteraceae	taxon_118	99	5	28	0	55	0	0	0	6	18	0	0	10	0	0	
Rhodobacteraceae	taxon_129	42	0	0	12	42	0	0	35	0	0	9	34	0	0	8	
Rhodobacteraceae	taxon_133	12	0	0	121	24	0	0	0	0	0	0	0	0	0	0	*
Rhodobacteraceae	taxon_145	24	0	11	37	0	0	16	31	8	0	0	0	0	0	0	
Rhodobacteraceae	taxon_157	46	0	0	19	0	0	0	0	0	0	0	14	15	0	6	
Rhodobacteraceae	taxon_241	0	0	0	0	0	0	5	27	0	4	0	0	0	0	0	
Rhodospirillales	taxon_187	0	0	0	0	0	0	0	0	0	0	0	39	13	0	11	
Unclassified	taxon_38	0	13	0	0	0	0	0	0	0	248	5	2086	0	11	517	
Unclassified	taxon_67	173	98	61	100	412	2	0	0	0	0	0	0	0	0	0	***
Unclassified	taxon_72	155	0	0	3	0	0	20	0	229	164	0	94	0	0	0	
Unclassified	taxon_73	317	9	7	68	0	20	8	23	0	61	6	27	79	0	20	
Unclassified	taxon_83	0	21	107	113	102	43	0	40	13	0	0	50	8	3	0	
Unclassified	taxon_86	433	0	17	15	0	0	0	0	0	0	0	0	0	0	0	*

Table S3.4 (cont.):

Unclassified	taxon_119	0	0	0	0	0	0	68	0	3	147	0	0	0	0	0	*
Unclassified	taxon_123	43	0	0	15	0	5	2	0	66	64	0	0	0	0	0	
Unclassified	taxon_144	34	0	33	22	0	7	0	16	0	10	0	0	6	0	0	
Unclassified	taxon_149	20	0	0	0	58	3	0	0	12	20	0	0	0	0	0	
Unclassified	taxon_172	0	8	6	0	20	6	8	0	0	16	0	0	17	0	0	
Staphylococcus sp.	taxon_227	10	0	6	23	0	0	0	0	0	0	0	0	0	0	0	
Sulfitobacter sp.	taxon_116	41	9	6	25	0	0	7	18	47	22	0	35	0	13	0	
Tepidibacter mesophilus	taxon_33	553	168	401	1403	638	0	0	0	0	13	0	0	0	0	0	***
Thalassospira sp.	taxon_82	66	13	36	159	0	0	11	52	69	0	18	11	60	12	0	
Thalassospira sp.	taxon_141	12	0	10	15	29	0	0	0	0	0	0	50	19	0	0	
Thalassospira xiamenensis	taxon_178	23	0	18	30	0	0	0	0	0	0	0	0	0	0	0	
Thalassotalea sp.	taxon_34	652	58	356	285	313	102	102	274	338	141	112	241	71	54	0	
Thalassotalea ganghwensis	taxon_10	3031	457	1862	1556	1710	611	545	1718	1763	744	562	1188	529	492	0	
Vibrio sp.	taxon_13	4753	536	872	1837	1637	130	45	105	1478	659	121	654	125	48	0	
Vibrio crosai	taxon_11	4427	3790	1512	3078	2361	48	16	73	77	156	46	400	477	0	28	
Vibrio crosai	taxon_39	813	636	268	517	367	0	0	61	24	0	0	82	53	0	0	**
Vibrio crosai	taxon_42	769	547	293	445	404	0	0	0	0	0	0	64	49	0	0	***
Vibrio sinaloensis	taxon_43	626	579	343	404	382	0	0	22	0	0	0	38	29	0	0	***
Vibrio sinaloensis	taxon_44	688	556	235	399	328	0	0	33	0	0	0	45	106	14	0	***
Vibrionaceae	taxon_19	3247	374	599	1534	1232	48	0	100	759	50	0	131	12	0	0	**
Vibrionaceae	taxon_20	3395	431	565	1440	1078	0	29	98	725	75	0	0	0	0	0	***
Vibrionaceae	taxon_55	274	63	306	490	162	0	0	0	0	0	0	0	10	0	0	***
Vibrionaceae	taxon_70	198	24	22	89	84	8	0	9	106	68	19	78	0	0	0	*
Zhongshania sp.	taxon_200	14	5	4	0	0	0	0	16	0	16	0	0	0	0	0	

Chapter 4

Table S4.1: Oxygen evolution at seven irradiances to determine saturating irradiance for symbiotic anemones

Sample	0 µmol photons (mg O_2 h^{-1})	20 µmol photons (mg O_2 h^{-1})	50 µmol photons (mg O_2 h^{-1})	100 µmol photons (mg O_2 h^{-1})	250 µmol photons (mg O_2 h^{-1})	400 µmol photons (mg O_2 h^{-1})	1000 µmol photons (mg O_2 h^{-1})	Saturating Irradiance (E_k; µmol photons)
Biorep 1	-0.0358	0.0207	0.0457	0.0650	0.0630	0.0511	0.0372	173.423
Biorep 2	-0.0725	0.0243	0.0997	0.1406	0.0981	0.0310	0.0469	108.744
Biorep 3	-0.1104	0.0532	0.1273	0.1674	0.0851	0.0311	0.0356	87.829
Biorep 4	-0.0468	0.0116	0.0450	0.1008	0.0991	0.0511	0.0372	156.998

Table S4.2: Differentially abundant BVOCs (< 0.05) detected across aposymbiotic anemones at 1) 25 °C (control); 2) 30°C (mid) and 3) 33.5 °C (high)

BVOC	logFC	AveExpr	P.Value	adj.P.Val	label	Higher in
2,7,10-trimethyldodecane	10.69152	7.526642	4.78E-05	0.006171	control vs heat	heat
2-Phenyl-3-methyl-pyrrolo(2,3-b)pyrazine	15.81566	10.73306	3.14E-08	4.05E-06	mid vs heat	mid
Napthalene	9.450171	8.982321	0.000808	0.029965	mid vs heat	mid
6-Methyl-triazolo(2,3-b)(1,2,4)-triazine	9.169106	8.50222	0.000929	0.029965	mid vs heat	mid
Di-tert-butyl peroxide	9.004638	8.819416	0.001191	0.029965	mid vs heat	mid
1,2-Dichloroethane	8.969308	8.547841	0.001398	0.029965	mid vs heat	mid
Acetone	9.284798	10.1941	0.001613	0.029965	mid vs heat	mid
Dibromomethane	8.744609	8.667974	0.001626	0.029965	mid vs heat	mid
2,7,10-trimethyldodecane	-8.27221	7.526642	0.002938	0.037705	mid vs heat	heat
1,2,3-Trimethylindene	8.176538	6.933994	0.002946	0.037705	mid vs heat	mid
1,2,4-Trimethylbenzene	8.332963	8.879407	0.003211	0.037705	mid vs heat	mid
2-Butanone	8.249844	8.229035	0.003215	0.037705	mid vs heat	mid
2-Amino-5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidine	8.116112	8.033807	0.004291	0.045742	mid vs heat	mid
Hexadecane	-7.04345	6.547053	0.00461	0.045742	mid vs heat	heat
2-Propenylbenzene	7.643879	7.977675	0.005344	0.049244	mid vs heat	mid

Table S4.3: Differentially abundant BVOCs (<0.05) detected across symbiotic anemones at 1) 25 °C (control); 2) 30°C (mid) and 3) 33.5 °C (high)

BVOC	logFC	AveExpr	P.Value	adj.P.Val	label	Higher in
Dimethyl sulphide	9.974351	14.976	5.17E-06	0.000517	control vs heat	heat
1-(2-Pyridyl)piperazine	8.197696	7.415443	0.000153	0.007628	control vs heat	heat
1-Iodododecane	7.03342	12.80556	0.001114	0.037141	control vs heat	heat

1-(2-Pyridyl)piperazine	-8.37793	7.415443	0.000248	0.017247	mid vs heat	heat
2,7,10-trimethyldodecane	-8.72061	6.225604	0.000378	0.017247	mid vs heat	heat
Di-tert-butyl peroxide	7.938375	7.262856	0.000574	0.017247	mid vs heat	mid
Dimethyl sulphide	-5.703	14.976	0.00069	0.017247	mid vs heat	heat
Eucalyptol	-8.16591	5.929439	0.001045	0.020892	mid vs heat	heat
Methyl N-hydroxybenzenecarboximidoate	-7.90354	7.151814	0.001706	0.02844	mid vs heat	heat

Table S4.4: Differentially abundant microbes (<0.05) detected across aposymbiotic anemones at 1) 25 °C (control); 2) 30°C (mid) and 3) 33.5 °C (high)

name	taxon_ID	logFC	adj.P.Val	label	Higher in
Tenacibaculum	taxon_25	10.58784	5.26E-06	control vs heat	heat
Flavobacteriaceae	taxon_66	-7.77758	5.26E-06	control vs heat	control
Crocinitomicaceae	taxon_42	-8.47409	2.19E-05	control vs heat	control
Flavobacteriaceae	taxon_32	-9.15157	5.66E-05	control vs heat	control
Polaribacter huanghezhanensis	taxon_137	-5.6785	0.000110599	control vs heat	control
Vibrionaceae	taxon_33	-3.10417	0.000183263	control vs heat	control
Oligoflexia	taxon_9	2.946239	0.000183263	control vs heat	heat
Bacteroidetes	taxon_139	-5.49465	0.000186907	control vs heat	control
Vibrionaceae	taxon_16	1.84507	0.000234281	control vs heat	heat
Flavobacteriaceae	taxon_53	-7.42335	0.000283189	control vs heat	control
Gammaproteobacteria	taxon_36	-2.70881	0.000487912	control vs heat	control
Gammaproteobacteria	taxon_45	-2.24465	0.000582246	control vs heat	control
Vibrionaceae	taxon_22	-1.79335	0.000641333	control vs heat	control
Peptostreptococcaceae	taxon_39	5.210716	0.000641333	control vs heat	heat
Vibrionaceae	taxon_12	1.526581	0.000641333	control vs heat	heat
Vibrio crosai	taxon_26	1.998094	0.000798566	control vs heat	heat
Thalassotalea ganghwensis	taxon_4	-1.68574	0.001523215	control vs heat	control
Vibrio sinaloensis	taxon_90	4.430225	0.003544444	control vs heat	heat
Crocinitomicaceae	taxon_2	-7.30033	0.004051385	control vs heat	control
root	taxon_82	-4.13577	0.004409044	control vs heat	control
Vibrio crosai	taxon_69	3.732896	0.00521942	control vs heat	heat
Marinilabiliales	taxon_18	-4.47739	0.006500221	control vs heat	control
Firmicutes	taxon_70	3.322814	0.01363509	control vs heat	heat
Owenweeksia	taxon_57	-4.73853	0.015498665	control vs heat	control
root	taxon_63	3.905587	0.015942125	control vs heat	heat
Aliivibrio finisterrensis	taxon_74	3.225584	0.015942125	control vs heat	heat
Tepidibacter mesophilus	taxon_77	-4.92674	0.019121579	control vs heat	control
Terasakiella pusilla	taxon_56	1.962625	0.021582226	control vs heat	heat
root	taxon_94	4.321121	0.025103223	control vs heat	heat
Cohaesibacter	taxon_71	3.467567	0.025103223	control vs heat	heat
Thalassotalea	taxon_28	-1.67868	0.028029448	control vs heat	control

Peptostreptococcaceae	taxon_39	7.103493	0.00014467	control vs mid	mid
Crocinitomicaceae	taxon_42	-7.56628	0.00014467	control vs mid	control
Flavobacteriaceae	taxon_66	-5.61417	0.000251547	control vs mid	control
Gammaproteobacteria	taxon_45	-3.35994	0.000264673	control vs mid	control
Gammaproteobacteria	taxon_36	-3.36534	0.000541831	control vs mid	control
Polaribacter huanghezhanensis	taxon_137	-4.77069	0.000696582	control vs mid	control
Flavobacteriaceae	taxon_89	5.859259	0.000788227	control vs mid	mid
Gammaproteobacteria	taxon_75	5.736169	0.000886689	control vs mid	mid
Bacteroidetes	taxon_139	-4.58684	0.001202606	control vs mid	control
Arcobacter	taxon_38	-4.77816	0.00129387	control vs mid	control
Flavobacteriaceae	taxon_53	-6.18225	0.001774387	control vs mid	control
Tenacibaculum	taxon_25	6.278204	0.003251406	control vs mid	mid
Oligoflexia	taxon_9	2.135455	0.005483937	control vs mid	mid
Peptostreptococcaceae	taxon_60	4.673446	0.008400103	control vs mid	mid
Vibrionaceae	taxon_12	1.192562	0.010968532	control vs mid	mid
root	taxon_82	-3.78296	0.010968532	control vs mid	control
Flavobacteriaceae	taxon_50	-3.7843	0.010968532	control vs mid	control
Vibrionaceae	taxon_22	-1.17658	0.016531443	control vs mid	control
Vibrionaceae	taxon_33	-1.31218	0.018074857	control vs mid	control
Ferrimonas	taxon_44	1.037577	0.030463484	control vs mid	mid
Gammaproteobacteria	taxon_52	-1.7033	0.033080524	control vs mid	control
Vibrionaceae	taxon_16	1.03522	0.033080524	control vs mid	mid
Flavobacteriaceae	taxon_32	-3.48752	0.034021307	control vs mid	control
root	taxon_63	3.747781	0.034021307	control vs mid	mid
Rhodobacteraceae	taxon_59	-2.1438	0.046226617	control vs mid	control
Flavobacteriaceae	taxon_89	5.662998	0.005796412	mid vs heat	mid
Gammaproteobacteria	taxon_52	-2.72427	0.005796412	mid vs heat	heat
Tenacibaculum	taxon_25	-4.30964	0.007272073	mid vs heat	heat
Crocinitomicaceae	taxon_2	8.161344	0.007272073	mid vs heat	mid
Arcobacter	taxon_38	-4.14078	0.013564334	mid vs heat	heat
Vibrio crosai	taxon_26	-1.6688	0.035332238	mid vs heat	heat
Flavobacteriaceae	taxon_32	5.664053	0.035332238	mid vs heat	mid
Peptostreptococcaceae	taxon_39	1.892777	0.035332238	mid vs heat	mid
Thalassotalea ganghwensis	taxon_4	1.31872	0.035332238	mid vs heat	mid
Vibrionaceae	taxon_33	1.791984	0.049809398	mid vs heat	mid

Table S4.5: Differentially abundant microbes (<0.05) detected across symbiotic anemones at 1) 25 °C (control); 2) 30°C (mid) and 3) 33.5 °C (high)

Name	**taxon_ID**	**logFC**	**adj.P.Val**	**label**	**Higher in**
Crocinitomicaceae	taxon_2	-7.90551	2.99E-07	control vs heat	control
Cytophagia	taxon_86	-6.42188	7.56E-06	control vs heat	control
Flavobacteriales	taxon_88	-6.66614	9.87E-06	control vs heat	control
Cytophagales	taxon_149	-6.33717	9.88E-06	control vs heat	control

Flavobacteriaceae	taxon_65	-6.19176	1.53E-05	control vs heat	control
Oligoflexia	taxon_9	5.469811	1.53E-05	control vs heat	heat
Rhodobacteraceae	taxon_143	-5.54192	0.000149994	control vs heat	control
Alteromonas	taxon_47	4.876615	0.000149994	control vs heat	heat
Vibrio crosai	taxon_26	4.676575	0.000155242	control vs heat	heat
Vibrio	taxon_10	4.668368	0.000167218	control vs heat	heat
Chlamydiia	taxon_214	-5.34852	0.000370846	control vs heat	control
Flavobacteriia	taxon_81	-5.29383	0.00054085	control vs heat	control
Alteromonas	taxon_14	4.433354	0.00054085	control vs heat	heat
root	taxon_189	-4.89383	0.0009761	control vs heat	control
Gammaproteobacteria	taxon_36	-4.62312	0.002076864	control vs heat	control
Gammaproteobacteria	taxon_5	2.67504	0.002095668	control vs heat	heat
Flavobacteriaceae	taxon_171	-4.65287	0.00230683	control vs heat	control
Proteobacteria	taxon_222	-4.5194	0.002647852	control vs heat	control
Alteromonas australica	taxon_13	3.738172	0.002946272	control vs heat	heat
Haliscomenobacteraceae	taxon_83	3.862584	0.006323184	control vs heat	heat
Cytophagia	taxon_326	-4.12896	0.006323184	control vs heat	control
Proteobacteria	taxon_275	-4.03008	0.007541447	control vs heat	control
root	taxon_68	-3.8232	0.007541447	control vs heat	control
Rhodobacteraceae	taxon_27	3.711209	0.008072814	control vs heat	heat
Alphaproteobacteria	taxon_80	3.299819	0.011450343	control vs heat	heat
Alteromonas simiduii	taxon_72	3.42617	0.014056082	control vs heat	heat
root	taxon_174	-3.67367	0.014056082	control vs heat	control
Tenacibaculum	taxon_25	-2.46686	0.017333486	control vs heat	control
Limimaricola	taxon_43	2.457446	0.034165977	control vs heat	heat
Rhodobacteraceae	taxon_64	-2.97126	0.03950011	control vs heat	control
Cytophagia	taxon_86	-5.55033	0.000132033	control vs mid	control
Vibrio	taxon_10	5.216039	0.000935404	control vs mid	mid
Flavobacteriales	taxon_88	-4.71845	0.003427665	control vs mid	control
Cytophagales	taxon_149	-4.38948	0.004086986	control vs mid	control
Oligoflexia	taxon_9	4.902661	0.004510665	control vs mid	mid
Flavobacteriaceae	taxon_65	-3.95199	0.013732482	control vs mid	control
Crocinitomicaceae	taxon_2	-4.18786	0.014496637	control vs mid	control
Gammaproteobacteria	taxon_36	-3.87638	0.016718098	control vs mid	control
Rhodobacteraceae	taxon_143	-3.59424	0.023691057	control vs mid	control
Rhodobacteraceae	taxon_64	-3.59183	0.027046478	control vs mid	control
Mesoflavibacter	taxon_1	-2.19039	0.032293399	control vs mid	control
Rhodobacteraceae	taxon_85	-3.39925	0.036989051	control vs mid	control
Chlamydiia	taxon_214	-3.40084	0.037792791	control vs mid	control
Flavobacteriia	taxon_81	-3.34614	0.046149873	control vs mid	control
Lewinellaceae	taxon_49	3.788556	0.047884358	control vs mid	mid
Alteromonas	taxon_47	-4.01067	0.021433566	mid vs heat	heat
Alteromonas	taxon_14	-3.70726	0.029046591	mid vs heat	heat
Sphingomonas	taxon_242	4.45095	0.029046591	mid vs heat	mid

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Table S4.6: BVOCs detected throughout aposymbiotic dataset. All BVOCs (peak normalised to protein content) and their chemical classes that were detected in aposymbiotic anemones at three different temperature treatments (control: 25 °C, sub-bleaching: 30 °C and bleaching: 33.5 °C). BVOCs had to be detected in at least three replicates in at least one temperature treatment to be included. Chemical class was determined based on the molecule's functional group(s). Significance was determined using differential abundance testing and the number of asterisks denotes the size of the adjusted p-value: *<0.05, **<0.01, ***<0.001.

BVOC	Control Aposymbiotic						Mid Aposymbiotic					Heat Aposymbiotic						Functional group	Significance
(1-Methylethyl)-benzene	2.E+03	9.E+02	2.E+03	0	0	0	3.E+03	1.E+03	0	0	3.E+01	5.E+02	3.E+01	0	2.E+01	0	0	Aromatic compound	
(E)-1-Propenylaziridine	0	3.E+02	4.E+02	0	0	8.E+02	0	0	2.E+02	0	0	0	0	0	6.E+01	0	3.E+02	Nitrogen containing compound	
1-(2-Pyridyl)piperazine	0	0	0	0	0	3.E+02	0	4.E+02	1.E+03	0	0	7.E+01	1.E+02	0	1.E+03	0	2.E+02	Nitrogen containing compound	
1,1,2,2,3,3-Hexamethylindane	0	2.E+02	2.E+02	0	0	8.E+00	2.E+02	0	0	0	0	0	0	0	4.E+01	0	0	Aromatic compound	
1,1-dimethyl ester butanoic acid	0	0	0	0	9.E+01	0	1.E+03	9.E+02	0	0	0	2.E+02	1.E+02	0	4.E+02	0	0	Ester	
1,2,3-Trimethylbenzene	5.E+03	6.E+03	4.E+03	0	0	0	4.E+03	2.E+04	2.E+03	0	0	0	0	0	0	0	0	Aromatic compound	
1,2,3-Trimethylindene	0	3.E+02	0	0	1.E+01	0	7.E+02	8.E+02	2.E+02	8.E+01	2.E+02	0	0	0	0	0	0	Aromatic compound	*
1,2,4-Trimethylbenzene	2.E+04	2.E+04	2.E+04	0	0	0	2.E+04	7.E+04	1.E+04	0	0	0	0	0	0	0	0	Aromatic compound	*
1,2-Dichloroethane	2.E+03	3.E+03	5.E+03	0	0	0	5.E+03	2.E+04	7.E+02	0	5.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	*
1,2-Dimethylhydrindene	1.E+02	2.E+02	1.E+02	0	0	0	2.E+02	4.E+02	0	0	0	0	0	0	0	0	0	Aromatic compound	
Ethylbenzene	1.E+03	1.E+03	1.E+03	0	3.E+02	0	7.E+02	7.E+02	0	0	0	0	0	0	0	0	0	Aromatic compound	
1,3-Dimethylbenzene	3.E+03	3.E+03	3.E+03	0	0	0	4.E+03	5.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
1,4-Dioxaspiro[4,5]decane	2.E+03	3.E+03	3.E+03	0	0	0	5.E+03	7.E+03	9.E+01	0	0	0	0	0	0	0	0	Ether	
1,6,7-Trimethylnapthalene	6.E+02	6.E+02	2.E+02	7.E+00	0	2.E+02	0	0	0	0	0	0	0	0	1.E+02	0	3.E+02	Aromatic compound	
1-Acetyl-4-(4-propylcyclohexyl)-benzene	0	2.E+02	1.E+02	6.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	Ketone	
1-Ethyl-2,4-dimethylbenzene	1.E+03	9.E+02	1.E+02	0	0	0	3.E+02	3.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
1-Ethyl-2-methylbenzene	2.E+03	2.E+03	1.E+03	0	0	0	1.E+03	4.E+03	2.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
1-ethyl-4-methylbenzene	4.E+03	3.E+03	3.E+03	0	0	0	3.E+03	1.E+04	3.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
1H-Indane, 2,3-dihydro-4,7-dimethyl-	3.E+02	1.E+02	3.E+01	0	0	0	2.E+02	5.E+02	0	0	0	0	0	0	0	0	0	Aromatic compound	
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	0	4.E+02	0	0	0	0	4.E+02	3.E+02	0	0	2.E+02	0	0	0	0	0	0	Aromatic compound	
1H-Indene, 2,3-dihydro-4,7-dimethyl-	0	5.E+01	3.E+01	0	0	0	2.E+02	1.E+02	2.E+01	0	1.E+01	1.E+01	0	0	0	0	0	Aromatic compound	
1H-Indole-5-carbonitrile	1.E+04	4.E+03	4.E+03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Nitrogen containing compound	
1-Iodododecane	2.E+04	6.E+04	0	0	0	0	5.E+04	2.E+04	0	0	2.E+04	6.E+03	1.E+04	1.E+04	0	2.E+03	0	Halogenated hydrocarbon	
1-Isopropyl-3,4-dimethyl-2-pyrazoline	4.E+02	3.E+02	3.E+02	0	0	0	1.E+03	3.E+03	0	0	0	0	0	0	0	0	0	Nitrogen containing compound	
1-Methoxy-2,3-dimethylaziridine	2.E+02	3.E+02	5.E+02	0	0	0	7.E+01	4.E+01	0	0	0	0	0	0	1.E+02	0	0	DFG	
1-Methyl-1H-2,3-benzodiazepine	0	0	0	0	0	0	4.E+02	0	0	0	5.E+01	3.E+01	7.E+01	0	7.E+01	0	0	Nitrogen containing compound	
1-Methyl-1H-pyrrole	0	4.E+02	6.E+02	0	5.E+02	0	1.E+03	1.E+03	0	0	4.E+02	0	0	0	1.E+03	0	0	Nitrogen containing compound	
1-Methyl-2-propylbenzene	1.E+03	6.E+02	1.E+02	0	0	0	0	1.E+03	0	0	0	0	0	0	4.E+02	0	0	Aromatic compound	
1-Methylethyl ester dodenanoic acid	4.E+02	7.E+01	0	0	0	3.E+02	0	0	0	0	0	0	0	0	0	0	3.E+02	Ester	
1-Nitro-4-(phenylmethoxy)-benzene	1.E+03	0	7.E+02	0	2.E+02	0	0	0	0	0	0	0	0	0	0	0	9.E+01	DFG	
1-Phenyl-1,2-propanediol	4.E+02	2.E+02	0	0	9.E+01	0	0	0	0	0	0	0	0	0	2.E+02	0	0	Alcohol	
2(3H)-Benzoxazolone	2.E+02	3.E+02	2.E+02	0	0	0	2.E+02	5.E+02	7.E+01	0	0	0	0	0	0	0	0	DFG	
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	9.E+02	6.E+02	1.E+03	0	0	2.E+02	4.E+02	0	0	0	0	0	0	0	0	0	0	Ester	

Table S4.6 (cont.):

2,2-Dibromo-1-methyl-cyclopropanecarboxylic acid hydrazide	0	0	3.E+01	0	0	0	3.E+01	3.E+01	3.E+00	0	0	0	0	0	0	0	0	DFG	
2,3-Dihydro-5-methyl-1H-indene	7.E+02	7.E+02	6.E+02	0	0	0	4.E+02	2.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
2,4-Dimethylstyrene	1.E+03	1.E+03	6.E+02	0	0	0	9.E+02	3.E+03	3.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
2,7,10-trimethyldodecane	0	0	0	0	0	0	3.E+03	0	0	0	0	1.E+03	2.E+03	2.E+03	0	1.E+04	9.E+01	Alkane	***
2,7-Dimethylnapthalene	1.E+04	1.E+03	2.E+03	0	0	0	0	0	0	0	0	2.E+01	0	0	0	0	0	Aromatic compound	
2-[(1-(4-Methylphenyl)ethylidene)amino]benzonitrile	0	2.E+02	1.E+02	0	0	3.E+02	0	0	0	0	0	0	0	0	5.E+01	0	7.E+02	Nitrogen containing compound	
2-[4-(1,1-dimethylpropyl)phenoxy]-ethanol	0	0	2.E+02	0	0	2.E+01	1.E+02	3.E+02	2.E+02	0	0	0	0	0	0	0	5.E+02	DFG	
2-Acetyl-5-methylthiophene	8.E+02	7.E+02	7.E+02	0	0	0	1.E+02	0	0	0	1.E+00	0	0	0	6.E+00	0	0	DFG	
2-Amino-5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidine	0	4.E+02	0	0	0	2.E+02	1.E+03	2.E+03	6.E+02	4.E+02	4.E+02	0	0	0	0	0	8.E+01	Nitrogen containing compound	*
2-Butanone	3.E+03	3.E+03	0	0	1.E+03	0	0	3.E+03	1.E+03	8.E+02	1.E+03	0	0	0	0	0	0	Ketone	*
2-Chloro-2,2-difluoro-1-phenylethanone	1.E+03	7.E+02	0	0	0	6.E+02	4.E+02	3.E+02	5.E+02	0	0	0	0	0	0	0	4.E+02	DFG	
2-Ethenylnapthalene	6.E+03	2.E+03	2.E+03	0	0	0	0	0	0	0	0	4.E+02	0	0	0	0	0	Aromatic compound	
2-Ethyl-1-hexanol	2.E+03	4.E+03	2.E+02	0	5.E+02	0	0	0	0	0	0	0	0	0	0	0	6.E+02	Alcohol	
2-Ethylhexyl hexyl ester sulphurous acid	7.E+03	0	0	0	9.E+02	5.E+03	0	0	0	0	0	0	3.E+03	0	0	0	0	Sulphur containing compound	
2-Methoxy-1-(2-nitroethenyl)-3-(phenylmethoxy)-benzene	2.E+03	4.E+03	7.E+03	0	0	0	0	1.E+04	0	0	0	0	0	0	0	0	0	DFG	
2-Methoxyfuran	0	0	6.E+02	0	0	0	0	8.E+02	0	0	0	4.E+02	3.E+02	0	5.E+02	0	0	Ether	
2-Methyl-2-propanol	1.E+03	4.E+03	5.E+03	8.E+01	1.E+02	1.E+01	3.E+03	5.E+03	0	0	5.E+02	0	0	0	0	0	0	Alcohol	
2-Phenyl-3-methyl-pyrrolo(2,3-b)pyrazine	1.E+04	5.E+03	3.E+03	0	0	0	2.E+05	1.E+05	4.E+04	2.E+04	3.E+04	0	0	0	0	0	0	Nitrogen containing compound	***
2-Propenal	4.E+02	4.E+02	9.E+02	0	0	7.E+01	0	3.E+02	0	0	0	0	0	0	0	0	7.E+01	Ketone	
2-Propenylbenzene	5.E+02	2.E+03	1.E+03	0	0	0	1.E+03	5.E+03	6.E+02	0	3.E+02	0	0	0	0	0	0	Aromatic compound	*
2-tert-butyl-5-(2-methylprop-2-en-1-yl)cyclohexa-2,5-diene-1,4-dione	7.E+01	5.E+02	8.E+01	0	2.E+02	4.E+01	0	0	0	0	0	0	0	0	0	0	0	Ketone	
3,3,5-Trimethylcyclohexyl methacrylate	3.E+04	8.E+03	7.E+03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Ester	
3,4-Dimethyldihydrofuran-2,5-dione	0	0	0	0	0	0	0	3.E+02	0	0	6.E+00	0	7.E+01	0	4.E+02	0	1.E+02	Ester	
3-[(2,4-dichlorophenyl)methoxy]-benzaldehyde	0	0	0	0	2.E+02	0	1.E+02	2.E+02	0	0	8.E+01	0	0	0	0	0	0	DFG	
3-ethenyl-2-ethoxypyrazine	4.E+02	3.E+02	2.E+02	3.E+01	0	1.E+02	9.E+02	5.E+02	2.E+02	8.E+01	9.E+01	0	1.E+02	0	1.E+02	0	1.E+02	DFG	
3-Methoxypropanenitrile	3.E+03	1.E+03	5.E+03	0	1.E+03	0	0	3.E+03	0	0	0	0	1.E+03	0	2.E+03	0	0	DFG	
3-Methylfuran	5.E+02	2.E+02	0	0	8.E+01	0	2.E+01	2.E+00	0	0	0	0	0	0	3.E+02	0	0	Ether	
3-Tetradecyne	0	4.E+02	8.E+02	0	5.E+01	7.E+02	0	0	2.E+02	0	0	0	0	0	7.E+01	0	3.E+02	Alkyne	
4-(Phenylmethyl)benzeneethanamine	3.E+02	0	4.E+02	0	0	2.E+01	0	0	0	0	0	0	0	0	5.E+01	0	1.E+02	Nitrogen containing compound	
4-Azidoheptane	0	0	0	0	0	0	5.E+02	6.E+02	0	0	0	2.E+02	2.E+02	0	1.E+01	0	0	Nitrogen containing compound	
4-Ethylbenzoic acid, pentyl ester	4.E+02	4.E+02	5.E+02	0	0	0	2.E+03	1.E+03	0	0	0	0	0	0	0	0	0	Ester	
5-Undecyne	8.E+02	4.E+02	3.E+02	0	0	6.E+02	2.E+02	0	4.E+02	0	0	0	0	0	4.E+02	0	6.E+02	Alkyne	
6-Amino-1-hexanol, N,N-dimethyl-, methyl ether	0	0	0	0	0	0	6.E+01	4.E+02	1.E+03	0	0	0	0	0	1.E+02	0	0	DFG	
6-Methyl-triazolo(2,3-b)(1,2,4)-triazine	3.E+02	4.E+02	2.E+02	0	0	1.E+02	9.E+02	1.E+03	8.E+02	2.E+02	3.E+02	0	0	0	0	0	0	Nitrogen containing compound	*
Acetaldehyde	0	0	0	1.E+03	0	0	9.E+02	4.E+03	2.E+03	0	2.E+03	7.E+02	0	0	0	0	2.E+03	Aldehyde	

Table S4.6 (cont.):

Acetone	8.E+03	8.E+03	4.E+03	0	0	0	1.E+04	1.E+04	1.E+03	3.E+02	2.E+03	0	0	0	3.E+03	0	0	Aldehyde	*
Benzaldehyde	2.E+03	2.E+03	1.E+03	0	0	0	0	2.E+03	0	0	0	0	0	0	4.E+02	0	0	Aldehyde	
Benzene	1.E+03	1.E+03	5.E+02	0	0	0	9.E+02	1.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
Benzene, 1,3-bis(1-methylethyl)-	8.E+02	4.E+02	4.E+02	0	0	0	1.E+03	7.E+02	5.E+01	0	0	3.E+01	0	0	0	0	0	Aromatic compound	
Benzeneacetaldehyde	1.E+03	1.E+03	6.E+02	0	0	0	7.E+02	3.E+03	0	0	0	0	0	0	0	0	0	Aldehyde	
Benzeneacetic acid, a-amino-, methyl ester	0	2.E+02	2.E+02	8.E+01	0	4.E+00	2.E+02	0	1.E+02	0	0	0	1.E+02	0	2.E+02	0	0	DFG	
Bicyclo[4.2.0]octa-1,3,5-triene-7,8-dione	6.E+00	3.E+02	6.E+01	0	0	0	1.E+02	2.E+02	0	0	0	0	0	0	0	0	0	Aldehyde	
Bromochlorodifluoromethane	0	0	0	0	0	9.E+01	3.E+02	0	0	6.E+01	0	4.E+01	2.E+00	0	5.E+01	0	4.E+01	Halogenated hydrocarbon	
Bromodichloromethane	6.E+02	8.E+02	7.E+02	0	0	0	8.E+02	3.E+03	2.E+02	0	2.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	
Butanal	4.E+02	3.E+02	0	0	1.E+02	0	0	0	0	0	0	0	0	0	0	0	0	Aldehyde	
Chlorobenzene-d5	1.E+02	2.E+03	2.E+03	0	0	0	2.E+03	3.E+03	8.E+01	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
cis-Calamenene	1.E+03	9.E+02	8.E+02	2.E+02	0	0	8.E+02	1.E+03	2.E+02	0	0	0	0	0	0	0	1.E+02	Aromatic compound	
Cyanamide, (dimethylphenylphosphoranylidene)-	0	0	7.E+02	0	0	0	5.E+02	8.E+02	0	2.E+02	2.E+02	1.E+02	0	0	0	0	0	DFG	
Cyclohexanone	2.E+03	3.E+03	3.E+03	0	0	0	5.E+03	7.E+03	1.E+03	0	1.E+03	0	3.E+02	0	5.E+02	0	0	Ketone	
Cyclopropa[3,4]pentaleno[1,2-d][1,3]dioxole, 2a,2b,2c,5a,5b,5c-hexahydro-, (2aa,2ba,2ca,5aa,5ba,5ca)-	8.E+02	4.E+02	7.E+02	4.E+01	0	2.E+02	1.E+02	0	9.E+01	0	0	0	0	0	3.E+01	0	4.E+02	Ether	
Decanal	0	4.E+02	1.E+03	0	0	4.E+02	0	0	2.E+02	0	0	0	0	0	2.E+01	0	5.E+02	Aldehyde	
Dibromochloromethane	2.E+03	7.E+02	8.E+02	0	0	0	6.E+02	4.E+03	3.E+02	0	2.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	
Dibromomethane	4.E+02	7.E+02	1.E+03	0	3.E+02	0	6.E+02	1.E+03	1.E+02	2.E+02	5.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	*
Diethyl-, ethyl ester carbamodithioic acid	5.E+02	4.E+02	6.E+02	0	0	5.E+01	0	0	2.E+02	0	0	0	2.E+02	0	3.E+02	0	0	DFG	
Dimethyl disulphide	0	2.E+02	3.E+02	0	2.E+03	0	0	4.E+02	0	0	0	0	0	0	2.E+02	0	0	Sulphur containing compound	
Dimethyl-arsinic acid	5.E+02	2.E+02	2.E+02	0	3.E+01	2.E+02	0	6.E+02	4.E+01	0	0	3.E+00	3.E+01	0	1.E+02	0	0	DFG	
Diphenylmethane	8.E+02	3.E+02	2.E+02	0	0	0	5.E+01	7.E+01	0	0	0	0	0	0	0	0	3.E+00	Aromatic compound	
Di-tert-butyl peroxide	3.E+03	5.E+02	5.E+02	0	4.E+02	0	3.E+03	3.E+03	2.E+02	3.E+01	3.E+02	0	0	0	0	0	0	Ether	*
Heptane, 2,5,5-trimethyl	5.E+02	5.E+02	3.E+02	0	0	0	2.E+03	1.E+03	0	0	4.E+01	0	0	0	3.E+02	0	0	Alkane	
Hexadecane	0	4.E+03	0	0	0	0	0	0	0	0	0	0	0	2.E+04	0	2.E+03	4.E+03	Alkane	*
Hexanal	3.E+02	3.E+02	4.E+02	0	0	0	3.E+02	0	0	0	0	0	0	0	8.E+01	0	0	Aldehyde	
Histamine, N-acetyl-5-bromo-	1.E+02	2.E+01	9.E+01	0	0	0	0	1.E+02	0	0	0	0	0	0	1.E+01	0	0	DFG	
Homosalate	3.E+02	2.E+02	6.E+01	0	0	0	9.E+01	2.E+02	3.E+02	0	1.E+01	0	0	0	3.E+02	0	2.E+01	DFG	
Isocyanatomethane	0	2.E+03	0	1.E+03	0	0	3.E+03	0	8.E+02	3.E+02	4.E+02	7.E+02	3.E+02	0	6.E+02	0	4.E+02	DFG	
Isolongifoline	5.E+03	0	0	0	0	3.E+03	1.E+04	1.E+03	3.E+03	1.E+03	0	4.E+02	8.E+03	0	1.E+03	0	8.E+02	Alkene	
Methyl N-hydroxybenzenecarboximidoate	6.E+03	6.E+02	2.E+04	0	0	0	0	3.E+04	0	0	0	0	0	0	0	0	0	DFG	
Methylal	1.E+03	2.E+03	2.E+03	4.E+02	6.E+01	7.E+01	6.E+02	3.E+03	2.E+02	0	0	0	0	0	0	0	0	Ether	
Methylene chloride	0	2.E+02	2.E+02	1.E+02	0	4.E+01	0	4.E+02	0	0	6.E+00	6.E+01	0	0	5.E+01	0	0	Halogenated hydrocarbon	
Monoacetate tetraethylene glycol	4.E+01	2.E+02	2.E+02	0	0	0	0	3.E+02	0	0	0	0	0	0	0	0	0	DFG	
N-(4-methoxybenzyl)-thiazol-2-amine	1.E+02	1.E+02	2.E+02	0	0	0	6.E+01	4.E+02	1.E+02	0	0	0	0	0	0	0	0	DFG	
Naphtho[2,1-b]furan	2.E+02	3.E+02	7.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	1.E+02	Ether	
Napthalene	1.E+04	8.E+03	9.E+03	0	0	0	8.E+03	3.E+04	7.E+03	0	2.E+02	0	0	0	0	0	0	Aromatic compound	*
Neopentyl ester butyric acid	4.E+02	4.E+02	0	0	3.E+01	0	2.E+03	2.E+03	0	2.E+02	0	3.E+02	0	0	0	0	0	Ester	
n-Hexane	4.E+02	2.E+02	0	0	5.E+01	0	0	2.E+02	0	0	0	6.E+01	0	0	0	0	0	Alkane	

Table S4.6 (cont.):

N-Methylisatoic anhydride	7.E+02	5.E+02	1.E+03	0	0	0	0	0	2.E+02	0	0	0	0	0	4.E+02	0	0	DFG	
Nonanal	2.E+03	3.E+03	2.E+03	0	0	0	3.E+03	5.E+02	2.E+02	0	0	0	0	0	7.E+02	0	0	Aldehyde	
Octanal	8.E+01	7.E+02	1.E+03	0	0	0	2.E+03	5.E+02	0	0	0	0	0	0	1.E+02	0	0	Aldehyde	
o-Cymene_a	2.E+03	2.E+03	1.E+02	0	0	0	9.E+02	5.E+03	4.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
o-Cymene_c	1.E+03	5.E+02	9.E+02	0	0	0	4.E+02	2.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
o-Cymene_d	8.E+02	4.E+02	1.E+02	0	0	0	2.E+02	2.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
p-Xylene	2.E+03	2.E+03	2.E+03	0	0	0	3.E+03	6.E+03	2.E+01	0	0	0	0	0	0	0	0	Aromatic compound	
Pyrrolo(2,3-b)pyrazine	1.E+03	5.E+02	6.E+02	2.E+01	0	6.E+02	0	0	0	0	0	0	0	0	1.E+02	0	1.E+03	Nitrogen containing compound	
s-Triazole, 3-chloro-	0	0	0	0	0	3.E+02	5.E+02	7.E+02	0	1.E+02	1.E+02	0	0	0	0	0	4.E+02	DFG	
Styrene	2.E+03	2.E+03	1.E+03	0	0	0	2.E+03	4.E+03	2.E+02	0	4.E+02	4.E+02	9.E+01	0	1.E+02	0	0	Aromatic compound	
Tetrachloroethylene	7.E+01	8.E+01	0	0	0	0	5.E+01	7.E+01	0	0	2.E+00	4.E+01	3.E+01	0	2.E+01	0	0	Halogenated hydrocarbon	
Tetradecafluorohexane	2.E+02	3.E+02	2.E+02	3.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
Tetradecane	3.E+02	1.E+03	2.E+03	0	0	4.E+03	60216.14	0	0	0	0	0	0	0	1.E+03	2.E+02	1.E+03	Alkane	
Tetradecanoic acid, 10,13-dimethyl-, methyl ester	3.E+02	1.E+02	3.E+02	0	0	2.E+02	0	0	0	0	0	0	0	0	0	0	4.E+02	Ester	
Tolazoline acetate	2.E+02	2.E+02	2.E+02	3.E+00	0	0	1.E+02	2.E+02	7.E+01	3.E+01	2.E+01	5.E+01	4.E+01	0	0	0	0	DFG	
Toluene	8.E+03	8.E+03	9.E+03	0	0	0	1.E+04	1.E+04	2.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
Tribromomethane	3.E+03	2.E+03	7.E+02	0	0	0	2.E+03	9.E+03	6.E+02	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
Trichloromethane	9.E+02	1.E+03	1.E+03	0	0	0	1.E+03	4.E+03	4.E+02	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
Tridecane	0	1.E+03	0	0	0	2.E+03	1.E+03	0	4.E+02	0	4.E+02	0	0	0	0	0	0	Alkane	
UC_11.64	5.E+01	7.E+01	7.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Unclassified	
UC_11.82	2.E+02	4.E+02	3.E+02	0	0	0	0	9.E+01	0	0	0	4.E+01	6.E+01	0	0	0	0	Unclassified	
UC_17.19	9.E+01	1.E+02	1.E+02	0	2.E+01	0	0	0	0	0	0	0	0	0	0	0	0	Unclassified	
UC_40.63	6.E+03	4.E+03	3.E+03	0	0	0	0	0	0	0	0	1.E+02	0	0	1.E+02	0	0	Unclassified	
UC_42.05	2.E+03	7.E+02	4.E+02	0	0	0	4.E+03	3.E+03	7.E+02	3.E+02	4.E+02	5.E+02	0	0	0	0	1.E+01	Unclassified	
UC_42.51	0	0	0	0	0	0	9.E+01	2.E+02	0	3.E+01	0	0	8.E+01	0	6.E+01	0	0	Unclassified	
UC_42.58	5.E+02	4.E+02	0	0	0	0	6.E+02	4.E+02	9.E+01	0	0	0	7.E+01	0	8.E+01	0	0	Unclassified	
UC_43.08	8.E+02	9.E+02	1.E+03	2.E+02	0	4.E+01	0	2.E+02	2.E+02	0	0	2.E+02	3.E+02	0	4.E+02	0	4.E+01	Unclassified	
UC_43.20	4.E+02	5.E+02	2.E+02	0	0	0	0	0	0	0	0	0	0	0	2.E+02	0	0	Unclassified	
UC_43.63	3.E+02	3.E+02	8.E+02	2.E+02	4.E+01	0	0	0	1.E+02	0	0	0	0	0	0	0	0	Unclassified	
UC_43.76	4.E+00	0	7.E+01	0	0	0	0	0	0	0	0	1.E+01	4.E-01	0	2.E+01	0	0	Unclassified	
UC_43.82	2.E+02	1.E+02	5.E+02	0	0	8.E+01	0	0	4.E+00	0	0	0	0	0	7.E+01	0	1.E+02	Unclassified	
UC_44.09	2.E+00	3.E+01	0	0	0	0	5.E+02	5.E+02	2.E+02	0	0	0	0	0	0	0	0	Unclassified	
UC_44.34	3.E+02	0	0	4.E+00	0	2.E+02	0	2.E+02	2.E+02	0	0	0	1.E+02	0	4.E+02	0	0	Unclassified	
UC_44.56	3.E+02	0	2.E+02	0	0	2.E+02	4.E+02	6.E+02	3.E+02	2.E+02	1.E+02	0	0	0	6.E+01	0	0	Unclassified	
UC_45.57	1.E+03	0	6.E+01	0	0	5.E+01	6.E+02	5.E+02	3.E+02	0	1.E+02	0	0	0	0	0	3.E+02	Unclassified	
UC_45.72	5.E+02	5.E+02	0	0	5.E+01	0	4.E+02	1.E+02	4.E+01	0	0	1.E+02	3.E+01	0	2.E+02	0	0	Unclassified	
UC_45.88	0	2.E+02	0	3.E+01	0	0	1.E+02	3.E+02	6.E+01	0	0	0	2.E+01	0	3.E+01	0	1.E+02	Unclassified	
UC_45.93	3.E+02	3.E+02	4.E+02	0	4.E+01	2.E+02	0	2.E+02	2.E+02	0	0	0	0	0	3.E+02	0	0	Unclassified	
UC_46.33	2.E+03	2.E+03	1.E+03	0	8.E+01	0	4.E+03	0	1.E+03	0	0	2.E+02	0	0	0	0	0	Unclassified	
UC_46.80	0	0	0	0	1.E+02	0	0	0	0	0	0	0	0	7.E+01	2.E+02	0	2.E+02	Unclassified	
UC_9.22	6.E+03	6.E+03	5.E+03	0	0	0	0	0	0	0	0	0	0	0	1.E+03	0	0	Unclassified	

Table S4.7: BVOCs detected throughout symbiotic dataset. All BVOCs (peak normalised to protein content) and their chemical classes that were detected in symbiotic anemones at three different temperature treatments (control: 25 °C, sub-bleaching: 30 °C and bleaching: 33.5 °C). BVOCs had to be detected in at least three replicates in at least one temperature condition to be included. Chemical class was determined based on the molecule's functional group(s). Significance was determined using differential abundance testing and the number of asterisks denotes the size of the adjusted p-value: *<0.05, **<0.01, ***<0.001.

BVOC	Control Aposymbiotic						Mid Aposymbiotic					Heat Aposymbiotic						Functional group	Significance
(1-Methylethyl)-benzene	2.E+03	9.E+02	2.E+03	0	0	0	3.E+03	1.E+03	0	0	3.E+01	5.E+02	3.E+01	0	2.E+01	0	0	Aromatic compound	
(E)-1-Propenylaziridine	0	3.E+02	4.E+02	0	0	8.E+02	0	0	2.E+02	0	0	0	0	0	6.E+01	0	3.E+02	Nitrogen containing compound	
1-(2-Pyridyl)piperazine	0	0	0	0	0	3.E+02	0	4.E+02	1.E+03	0	0	7.E+01	1.E+02	0	1.E+03	0	2.E+02	Nitrogen containing compound	
1,1,2,2,3,3-Hexamethylindane	0	2.E+02	2.E+02	0	0	8.E+00	2.E+02	0	0	0	0	0	0	0	4.E+01	0	0	Aromatic compound	
1,1-dimethyl ester butanoic acid	0	0	0	0	9.E+01	0	1.E+03	9.E+02	0	0	0	2.E+02	1.E+02	0	4.E+02	0	0	Ester	
1,2,3-Trimethylbenzene	5.E+03	6.E+03	4.E+03	0	0	0	4.E+03	2.E+04	2.E+03	0	0	0	0	0	0	0	0	Aromatic compound	
1,2,3-Trimethylindene	0	3.E+02	0	0	1.E+01	0	7.E+02	8.E+02	2.E+02	8.E+01	2.E+02	0	0	0	0	0	0	Aromatic compound	*
1,2,4-Trimethylbenzene	2.E+04	2.E+04	2.E+04	0	0	0	2.E+04	7.E+04	1.E+04	0	0	0	0	0	0	0	0	Aromatic compound	*
1,2-Dichloroethane	2.E+03	3.E+03	5.E+03	0	0	0	5.E+03	2.E+04	7.E+02	0	5.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	*
1,2-Dimethylhydrindene	1.E+02	2.E+02	1.E+02	0	0	0	2.E+02	4.E+02	0	0	0	0	0	0	0	0	0	Aromatic compound	
Ethylbenzene	1.E+03	1.E+03	1.E+03	0	3.E+02	0	7.E+02	7.E+02	0	0	0	0	0	0	0	0	0	Aromatic compound	
1,3-Dimethylbenzene	3.E+03	3.E+03	3.E+03	0	0	0	4.E+03	5.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
1,4-Dioxaspiro[4,5]decane	2.E+03	3.E+03	3.E+03	0	0	0	5.E+03	7.E+03	9.E+01	0	0	0	0	0	0	0	0	Ether	
1,6,7-Trimethylnapthalene	6.E+02	6.E+02	2.E+02	7.E+00	0	2.E+02	0	0	0	0	0	0	0	0	1.E+02	0	3.E+02	Aromatic compound	
1-Acetyl-4-(4-propylcyclohexyl)-benzene	0	2.E+02	1.E+02	6.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	Ketone	
1-Ethyl-2,4-dimethylbenzene	1.E+03	9.E+02	1.E+02	0	0	0	3.E+02	3.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
1-Ethyl-2-methylbenzene	2.E+03	2.E+03	1.E+03	0	0	0	1.E+03	4.E+03	2.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
1-ethyl-4-methylbenzene	4.E+03	3.E+03	3.E+03	0	0	0	3.E+03	1.E+04	3.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
1H-Indane, 2,3-dihydro-4,7-dimethyl-	3.E+02	1.E+02	3.E+01	0	0	0	2.E+02	5.E+02	0	0	0	0	0	0	0	0	0	Aromatic compound	
1H-Indene, 2,3-dihydro-1,1,3-trimethyl-	0	4.E+02	0	0	0	0	4.E+02	3.E+02	0	0	2.E+02	0	0	0	0	0	0	Aromatic compound	
1H-Indene, 2,3-dihydro-4,7-dimethyl-	0	5.E+01	3.E+01	0	0	0	2.E+02	1.E+02	2.E+01	0	1.E+01	1.E+01	0	0	0	0	0	Aromatic compound	
1H-Indole-5-carbonitrile	1.E+04	4.E+03	4.E+03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Nitrogen containing compound	
1-Iodododecane	2.E+04	6.E+04	0	0	0	0	5.E+04	2.E+04	0	0	2.E+04	6.E+03	1.E+04	1.E+04	0	2.E+03	0	Halogenated hydrocarbon	
1-Isopropyl-3,4-dimethyl-2-pyrazoline	4.E+02	3.E+02	3.E+02	0	0	0	1.E+03	3.E+03	0	0	0	0	0	0	0	0	0	Nitrogen containing compound	
1-Methoxy-2,3-dimethylaziridine	2.E+02	3.E+02	5.E+02	0	0	0	7.E+01	4.E+01	0	0	0	0	0	0	1.E+02	0	0	DFG	
1-Methyl-1H-2,3-benzodiazepine	0	0	0	0	0	0	4.E+02	0	0	0	5.E+01	3.E+01	7.E+01	0	7.E+01	0	0	Nitrogen containing compound	
1-Methyl-1H-pyrrole	0	4.E+02	6.E+02	0	5.E+02	0	1.E+03	1.E+03	0	0	4.E+02	0	0	0	1.E+03	0	0	Nitrogen containing compound	
1-Methyl-2-propylbenzene	1.E+03	6.E+02	1.E+02	0	0	0	0	1.E+03	0	0	0	0	0	0	4.E+02	0	0	Aromatic compound	
1-Methylethyl ester dodenanoic acid	4.E+02	7.E+01	0	0	0	3.E+02	0	0	0	0	0	0	0	0	0	0	3.E+02	Ester	
1-Nitro-4-(phenylmethoxy)-benzene	1.E+03	0	7.E+02	0	2.E+02	0	0	0	0	0	0	0	0	0	0	0	9.E+01	DFG	
1-Phenyl-1,2-propanediol	4.E+02	2.E+02	0	0	9.E+01	0	0	0	0	0	0	0	0	0	2.E+02	0	0	Alcohol	
2(3H)-Benzoxazolone	2.E+02	3.E+02	2.E+02	0	0	0	2.E+02	5.E+02	7.E+01	0	0	0	0	0	0	0	0	DFG	
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	9.E+02	6.E+02	1.E+03	0	0	2.E+02	4.E+02	0	0	0	0	0	0	0	0	0	0	Ester	
2,2-Dibromo-1-methyl-cyclopropanecarboxylic acid hydrazide	0	0	3.E+01	0	0	0	3.E+01	3.E+01	3.E+00	0	0	0	0	0	0	0	0	DFG	
2,3-Dihydro-5-methyl-1H-indene	7.E+02	7.E+02	6.E+02	0	0	0	4.E+02	2.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
2,4-Dimethylstyrene	1.E+03	1.E+03	6.E+02	0	0	0	9.E+02	3.E+03	3.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
2,7,10-trimethyldodecane	0	0	0	0	0	0	3.E+03	0	0	0	0	1.E+03	2.E+03	2.E+03	0	1.E+04	9.E+01	Alkane	***
2,7-Dimethylnapthalene	1.E+04	1.E+03	2.E+03	0	0	0	0	0	0	0	0	2.E+01	0	0	0	0	0	Aromatic compound	

Table S4.7 (cont.):

2-[(1-(4-Methylphenyl)ethylidene)amino]benzonitrile	0	2.E+02	1.E+02	0	0	3.E+02	0	0	0	0	0	0	0	0	5.E+01	0	7.E+02	Nitrogen containing compound	
2-[4-(1,1-dimethylpropyl)phenoxy]-ethanol	0	0	2.E+02	0	0	2.E+01	1.E+02	3.E+02	2.E+02	0	0	0	0	0	0	0	5.E+02	DFG	
2-Acetyl-5-methylthiophene	8.E+02	7.E+02	7.E+02	0	0	0	1.E+02	0	0	0	1.E+00	0	0	0	6.E+00	0	0	DFG	
2-Amino-5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidine	0	4.E+02	0	0	0	2.E+02	1.E+03	2.E+03	6.E+02	4.E+02	4.E+02	0	0	0	0	0	8.E+01	Nitrogen containing compound	*
2-Butanone	3.E+03	3.E+03	0	0	1.E+03	0	0	3.E+03	1.E+03	8.E+02	1.E+03	0	0	0	0	0	0	Ketone	*
2-Chloro-2,2-difluoro-1-phenylethanone	1.E+03	7.E+02	0	0	0	6.E+02	4.E+02	3.E+02	5.E+02	0	0	0	0	0	0	0	4.E+02	DFG	
2-Ethenylnapthalene	6.E+03	2.E+03	2.E+03	0	0	0	0	0	0	0	0	4.E+02	0	0	0	0	0	Aromatic compound	
2-Ethyl-1-hexanol	2.E+03	4.E+03	2.E+02	0	5.E+02	0	0	0	0	0	0	0	0	0	0	0	6.E+02	Alcohol	
2-Ethylhexyl hexyl ester sulphurous acid	7.E+03	0	0	0	9.E+02	5.E+03	0	0	0	0	0	0	3.E+03	0	0	0	0	Sulphur containing compound	
2-Methoxy-1-(2-nitroethenyl)-3-(phenylmethoxy)-benzene	2.E+03	4.E+03	7.E+03	0	0	0	0	1.E+04	0	0	0	0	0	0	0	0	0	DFG	
2-Methoxyfuran	0	0	6.E+02	0	0	0	0	8.E+02	0	0	0	4.E+02	3.E+02	0	5.E+02	0	0	Ether	
2-Methyl-2-propanol	1.E+03	4.E+03	5.E+03	8.E+01	1.E+02	1.E+01	3.E+03	5.E+03	0	0	5.E+02	0	0	0	0	0	0	Alcohol	
2-Phenyl-3-methyl-pyrrolo(2,3-b)pyrazine	1.E+04	5.E+03	3.E+03	0	0	0	2.E+05	1.E+05	4.E+04	2.E+04	3.E+04	0	0	0	0	0	0	Nitrogen containing compound	***
2-Propenal	4.E+02	4.E+02	9.E+02	0	0	7.E+01	0	3.E+02	0	0	0	0	0	0	0	0	7.E+01	Ketone	
2-Propenylbenzene	5.E+02	2.E+03	1.E+03	0	0	0	1.E+03	5.E+03	6.E+02	0	3.E+02	0	0	0	0	0	0	Aromatic compound	*
2-tert-butyl-5-(2-methylprop-2-en-1-yl)cyclohexa-2,5-diene-1,4-dione	7.E+01	5.E+02	8.E+01	0	2.E+02	4.E+01	0	0	0	0	0	0	0	0	0	0	0	Ketone	
3,3,5-Trimethylcyclohexyl methacrylate	3.E+04	8.E+03	7.E+03	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Ester	
3,4-Dimethyldihydrofuran-2,5-dione	0	0	0	0	0	0	0	3.E+02	0	0	6.E+00	0	7.E+01	0	4.E+02	0	1.E+02	Ester	
3-[(2,4-dichlorophenyl)methoxy]-benzaldehyde	0	0	0	0	2.E+02	0	1.E+02	2.E+02	0	0	8.E+01	0	0	0	0	0	0	DFG	
3-ethenyl-2-ethoxypyrazine	4.E+02	3.E+02	2.E+02	3.E+01	0	1.E+02	9.E+02	5.E+02	2.E+02	8.E+01	9.E+01	0	1.E+02	0	1.E+02	0	1.E+02	DFG	
3-Methoxypropanenitrile	3.E+03	1.E+03	5.E+03	0	1.E+03	0	0	3.E+03	0	0	0	0	1.E+03	0	2.E+03	0	0	DFG	
3-Methylfuran	5.E+02	2.E+02	0	0	8.E+01	0	2.E+01	2.E+00	0	0	0	0	0	0	3.E+02	0	0	Ether	
3-Tetradecyne	0	4.E+02	8.E+02	0	5.E+01	7.E+02	0	0	2.E+02	0	0	0	0	0	7.E+01	0	3.E+02	Alkyne	
4-(Phenylmethyl)benzeneethanamine	3.E+02	0	4.E+02	0	0	2.E+01	0	0	0	0	0	0	0	0	5.E+01	0	1.E+02	Nitrogen containing compound	
4-Azidoheptane	0	0	0	0	0	0	5.E+02	6.E+02	0	0	0	2.E+02	2.E+02	0	1.E+01	0	0	Nitrogen containing compound	
4-Ethylbenzoic acid, pentyl ester	4.E+02	4.E+02	5.E+02	0	0	0	2.E+03	1.E+03	0	0	0	0	0	0	0	0	0	Ester	
5-Undecyne	8.E+02	4.E+02	3.E+02	0	0	6.E+02	2.E+02	0	4.E+02	0	0	0	0	0	4.E+02	0	6.E+02	Alkyne	
6-Amino-1-hexanol, N,N-dimethyl-, methyl ether	0	0	0	0	0	0	6.E+01	4.E+02	1.E+03	0	0	0	0	0	1.E+02	0	0	DFG	
6-Methyl-triazolo(2,3-b)(1,2,4)-triazine	3.E+02	4.E+02	2.E+02	0	0	1.E+02	9.E+02	1.E+03	8.E+02	2.E+02	3.E+02	0	0	0	0	0	0	Nitrogen containing compound	*
Acetaldehyde	0	0	0	1.E+03	0	0	9.E+02	4.E+03	2.E+03	0	2.E+03	7.E+02	0	0	0	0	2.E+03	Aldehyde	
Acetone	8.E+03	8.E+03	4.E+03	0	0	0	1.E+04	1.E+04	1.E+03	3.E+02	2.E+03	0	0	0	3.E+03	0	0	Aldehyde	*
Benzaldehyde	2.E+03	2.E+03	1.E+03	0	0	0	0	2.E+03	0	0	0	0	0	0	4.E+02	0	0	Aldehyde	
Benzene	1.E+03	1.E+03	5.E+02	0	0	0	9.E+02	1.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
Benzene, 1,3-bis(1-methylethyl)-	8.E+02	4.E+02	4.E+02	0	0	0	1.E+03	7.E+02	5.E+01	0	0	3.E+01	0	0	0	0	0	Aromatic compound	
Benzeneacetaldehyde	1.E+03	1.E+03	6.E+02	0	0	0	7.E+02	3.E+03	0	0	0	0	0	0	0	0	0	Aldehyde	
Benzeneacetic acid, a-amino-, methyl ester	0	2.E+02	2.E+02	8.E+01	0	4.E+00	2.E+02	0	1.E+02	0	0	0	1.E+02	0	2.E+02	0	0	DFG	
Bicyclo[4.2.0]octa-1,3,5-triene-7,8-dione	6.E+00	3.E+02	6.E+01	0	0	0	1.E+02	2.E+02	0	0	0	0	0	0	0	0	0	Aldehyde	
Bromochlorodifluoromethane	0	0	0	0	0	9.E+01	3.E+02	0	0	6.E+01	0	4.E+01	2.E+00	0	5.E+01	0	4.E+01	Halogenated hydrocarbon	
Bromodichloromethane	6.E+02	8.E+02	7.E+02	0	0	0	8.E+02	3.E+03	2.E+02	0	2.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	

Table S4.7 (cont.):

Butanal	4.E+02	3.E+02	0	0	1.E+02	0	0	0	0	0	0	0	0	0	0	0	0	Aldehyde	
Chlorobenzene-d5	1.E+02	2.E+03	2.E+03	0	0	0	2.E+03	3.E+03	8.E+01	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
cis-Calamenene	1.E+03	9.E+02	8.E+02	2.E+02	0	0	8.E+02	1.E+03	2.E+02	0	0	0	0	0	0	0	1.E+02	Aromatic compound	
Cyanamide, (dimethylphenylphosphoranylidene)-	0	0	7.E+02	0	0	0	5.E+02	8.E+02	0	2.E+02	2.E+02	1.E+02	0	0	0	0	0	DFG	
Cyclohexanone	2.E+03	3.E+03	3.E+03	0	0	0	5.E+03	7.E+03	1.E+03	0	1.E+03	0	3.E+02	0	5.E+02	0	0	Ketone	
Cyclopropa[3,4]pentaleno[1,2-d][1,3]dioxole, 2a,2b,2c,5a,5b,5c-hexahydro-, (2aa,2ba,2ca,5aa,5ba,5ca)-	8.E+02	4.E+02	7.E+02	4.E+01	0	2.E+02	1.E+02	0	9.E+01	0	0	0	0	0	3.E+01	0	4.E+02	Ether	
Decanal	0	4.E+02	1.E+03	0	0	4.E+02	0	0	2.E+02	0	0	0	0	0	2.E+01	0	5.E+02	Aldehyde	
Dibromochloromethane	2.E+03	7.E+02	8.E+02	0	0	0	6.E+02	4.E+03	3.E+02	0	2.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	
Dibromomethane	4.E+02	7.E+02	1.E+03	0	3.E+02	0	6.E+02	1.E+03	1.E+02	2.E+02	5.E+02	0	0	0	0	0	0	Halogenated hydrocarbon	*
Diethyl-, ethyl ester carbamodithioic acid	5.E+02	4.E+02	6.E+02	0	0	5.E+01	0	0	2.E+02	0	0	0	2.E+02	0	3.E+02	0	0	DFG	
Dimethyl disulphide	0	2.E+02	3.E+02	0	2.E+03	0	0	4.E+02	0	0	0	0	0	0	2.E+02	0	0	Sulphur containing compound	
Dimethyl-arsinic acid	5.E+02	2.E+02	2.E+02	0	3.E+01	2.E+02	0	6.E+02	4.E+01	0	0	3.E+00	3.E+01	0	1.E+02	0	0	DFG	
Diphenylmethane	8.E+02	3.E+02	2.E+02	0	0	0	5.E+01	7.E+01	0	0	0	0	0	0	0	0	3.E+00	Aromatic compound	
Di-tert-butyl peroxide	3.E+03	5.E+02	5.E+02	0	4.E+02	0	3.E+03	3.E+03	2.E+02	3.E+01	3.E+02	0	0	0	0	0	0	Ether	*
Heptane, 2,5,5-trimethyl	5.E+02	5.E+02	3.E+02	0	0	0	2.E+03	1.E+03	0	0	4.E+01	0	0	0	3.E+02	0	0	Alkane	
Hexadecane	0	4.E+03	0	0	0	0	0	0	0	0	0	0	0	2.E+04	0	2.E+03	4.E+03	Alkane	*
Hexanal	3.E+02	3.E+02	4.E+02	0	0	0	3.E+02	0	0	0	0	0	0	0	8.E+01	0	0	Aldehyde	
Histamine, N-acetyl-5-bromo-	1.E+02	2.E+01	9.E+01	0	0	0	0	1.E+02	0	0	0	0	0	0	1.E+01	0	0	DFG	
Homosalate	3.E+02	2.E+02	6.E+01	0	0	0	9.E+01	2.E+02	3.E+02	0	1.E+01	0	0	0	3.E+02	0	2.E+01	DFG	
Isocyanatomethane	0	2.E+03	0	1.E+03	0	0	3.E+03	0	8.E+02	3.E+02	4.E+02	7.E+02	3.E+02	0	6.E+02	0	4.E+02	DFG	
Isolongifoline	5.E+03	0	0	0	0	3.E+03	1.E+04	1.E+03	3.E+03	1.E+03	0	4.E+02	8.E+03	0	1.E+03	0	8.E+02	Alkene	
Methyl N-hydroxybenzenecarboximidoate	6.E+03	6.E+02	2.E+04	0	0	0	0	3.E+04	0	0	0	0	0	0	0	0	0	DFG	
Methylal	1.E+03	2.E+03	2.E+03	4.E+02	6.E+01	7.E+01	6.E+02	3.E+03	2.E+02	0	0	0	0	0	0	0	0	Ether	
Methylene chloride	0	2.E+02	2.E+02	1.E+02	0	4.E+01	0	4.E+02	0	0	6.E+00	6.E+01	0	0	5.E+01	0	0	Halogenated hydrocarbon	
Monoacetate tetraethylene glycol	4.E+01	2.E+02	2.E+02	0	0	0	0	3.E+02	0	0	0	0	0	0	0	0	0	DFG	
N-(4-methoxybenzyl)-thiazol-2-amine	1.E+02	1.E+02	2.E+02	0	0	0	6.E+01	4.E+02	1.E+02	0	0	0	0	0	0	0	0	DFG	
Naphtho[2,1-b]furan	2.E+02	3.E+02	7.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	1.E+02	Ether	
Napthalene	1.E+04	8.E+03	9.E+03	0	0	0	8.E+03	3.E+04	7.E+03	0	2.E+02	0	0	0	0	0	0	Aromatic compound	*
Neopentyl ester butyric acid	4.E+02	4.E+02	0	0	3.E+01	0	2.E+03	2.E+03	0	2.E+02	0	3.E+02	0	0	0	0	0	Ester	
n-Hexane	4.E+02	2.E+02	0	0	5.E+01	0	0	2.E+02	0	0	0	6.E+01	0	0	0	0	0	Alkane	
N-Methylisatoic anhydride	7.E+02	5.E+02	1.E+03	0	0	0	0	0	2.E+02	0	0	0	0	0	4.E+02	0	0	DFG	
Nonanal	2.E+03	3.E+03	2.E+03	0	0	0	3.E+03	5.E+02	2.E+02	0	0	0	0	0	7.E+02	0	0	Aldehyde	
Octanal	8.E+01	7.E+02	1.E+03	0	0	0	2.E+03	5.E+02	0	0	0	0	0	0	1.E+02	0	0	Aldehyde	
o-Cymene_a	2.E+03	2.E+03	1.E+02	0	0	0	9.E+02	5.E+03	4.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
o-Cymene_c	1.E+03	5.E+02	9.E+02	0	0	0	4.E+02	2.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
o-Cymene_d	8.E+02	4.E+02	1.E+02	0	0	0	2.E+02	2.E+03	0	0	0	0	0	0	0	0	0	Aromatic compound	
p-Xylene	2.E+03	2.E+03	2.E+03	0	0	0	3.E+03	6.E+03	2.E+01	0	0	0	0	0	0	0	0	Aromatic compound	
Pyrrolo(2,3-b)pyrazine	1.E+03	5.E+02	6.E+02	2.E+01	0	6.E+02	0	0	0	0	0	0	0	0	1.E+02	0	1.E+03	Nitrogen containing compound	
s-Triazole, 3-chloro-	0	0	0	0	0	3.E+02	5.E+02	7.E+02	0	1.E+02	1.E+02	0	0	0	0	0	4.E+02	DFG	
Styrene	2.E+03	2.E+03	1.E+03	0	0	0	2.E+03	4.E+03	2.E+02	0	4.E+02	4.E+02	9.E+01	0	1.E+02	0	0	Aromatic compound	
Tetrachloroethylene	7.E+01	8.E+01	0	0	0	0	5.E+01	7.E+01	0	0	2.E+00	4.E+01	3.E+01	0	2.E+01	0	0	Halogenated hydrocarbon	

Table S4.7 (cont.):

Tetradecafluorohexane	2.E+02	3.E+02	2.E+02	3.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
Tetradecane	3.E+02	1.E+03	2.E+03	0	0	4.E+03	60216.14	0	0	0	0	0	0	0	1.E+03	2.E+02	1.E+03	Alkane	
Tetradecanoic acid, 10,13-dimethyl-, methyl ester	3.E+02	1.E+02	3.E+02	0	0	2.E+02	0	0	0	0	0	0	0	0	0	0	4.E+02	Ester	
Tolazoline acetate	2.E+02	2.E+02	2.E+02	3.E+00	0	0	1.E+02	2.E+02	7.E+01	3.E+01	2.E+01	5.E+01	4.E+01	0	0	0	0	DFG	
Toluene	8.E+03	8.E+03	9.E+03	0	0	0	1.E+04	1.E+04	2.E+02	0	0	0	0	0	0	0	0	Aromatic compound	
Tribromomethane	3.E+03	2.E+03	7.E+02	0	0	0	2.E+03	9.E+03	6.E+02	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
Trichloromethane	9.E+02	1.E+03	1.E+03	0	0	0	1.E+03	4.E+03	4.E+02	0	0	0	0	0	0	0	0	Halogenated hydrocarbon	
Tridecane	0	1.E+03	0	0	0	2.E+03	1.E+03	0	4.E+02	0	4.E+02	0	0	0	0	0	0	Alkane	
UC_11.64	5.E+01	7.E+01	7.E+01	0	0	0	0	0	0	0	0	0	0	0	0	0	0	Unclassified	
UC_11.82	2.E+02	4.E+02	3.E+02	0	0	0	0	9.E+01	0	0	0	4.E+01	6.E+01	0	0	0	0	Unclassified	
UC_17.19	9.E+01	1.E+02	1.E+02	0	2.E+01	0	0	0	0	0	0	0	0	0	0	0	0	Unclassified	
UC_40.63	6.E+03	4.E+03	3.E+03	0	0	0	0	0	0	0	0	1.E+02	0	0	1.E+02	0	0	Unclassified	
UC_42.05	2.E+03	7.E+02	4.E+02	0	0	0	4.E+03	3.E+03	7.E+02	3.E+02	4.E+02	5.E+02	0	0	0	0	1.E+01	Unclassified	
UC_42.51	0	0	0	0	0	0	9.E+01	2.E+02	0	3.E+01	0	0	8.E+01	0	6.E+01	0	0	Unclassified	
UC_42.58	5.E+02	4.E+02	0	0	0	0	6.E+02	4.E+02	9.E+01	0	0	0	7.E+01	0	8.E+01	0	0	Unclassified	
UC_43.08	8.E+02	9.E+02	1.E+03	2.E+02	0	4.E+01	0	2.E+02	2.E+02	0	0	2.E+02	3.E+02	0	4.E+02	0	4.E+01	Unclassified	
UC_43.20	4.E+02	5.E+02	2.E+02	0	0	0	0	0	0	0	0	0	0	0	2.E+02	0	0	Unclassified	
UC_43.63	3.E+02	3.E+02	8.E+02	2.E+02	4.E+01	0	0	0	1.E+02	0	0	0	0	0	0	0	0	Unclassified	
UC_43.76	4.E+00	0	7.E+01	0	0	0	0	0	0	0	0	1.E+01	4.E-01	0	2.E+01	0	0	Unclassified	
UC_43.82	2.E+02	1.E+02	5.E+02	0	0	8.E+01	0	0	4.E+00	0	0	0	0	0	7.E+01	0	1.E+02	Unclassified	
UC_44.09	2.E+00	3.E+01	0	0	0	0	5.E+02	5.E+02	2.E+02	0	0	0	0	0	0	0	0	Unclassified	
UC_44.34	3.E+02	0	0	4.E+00	0	2.E+02	0	2.E+02	2.E+02	0	0	0	1.E+02	0	4.E+02	0	0	Unclassified	
UC_44.56	3.E+02	0	2.E+02	0	0	2.E+02	4.E+02	6.E+02	3.E+02	2.E+02	1.E+02	0	0	0	6.E+01	0	0	Unclassified	
UC_45.57	1.E+03	0	6.E+01	0	0	5.E+01	6.E+02	5.E+02	3.E+02	0	1.E+02	0	0	0	0	0	3.E+02	Unclassified	
UC_45.72	5.E+02	5.E+02	0	0	5.E+01	0	4.E+02	1.E+02	4.E+01	0	0	1.E+02	3.E+01	0	2.E+02	0	0	Unclassified	
UC_45.88	0	2.E+02	0	3.E+01	0	0	1.E+02	3.E+02	6.E+01	0	0	0	2.E+01	0	3.E+01	0	1.E+02	Unclassified	
UC_45.93	3.E+02	3.E+02	4.E+02	0	4.E+01	2.E+02	0	2.E+02	2.E+02	0	0	0	0	0	3.E+02	0	0	Unclassified	
UC_46.33	2.E+03	2.E+03	1.E+03	0	8.E+01	0	4.E+03	0	1.E+03	0	0	2.E+02	0	0	0	0	0	Unclassified	
UC_46.80	0	0	0	0	1.E+02	0	0	0	0	0	0	0	0	7.E+01	2.E+02	0	2.E+02	Unclassified	
UC_9.22	6.E+03	6.E+03	5.E+03	0	0	0	0	0	0	0	0	0	0	0	1.E+03	0	0	Unclassified	

Chapter 5

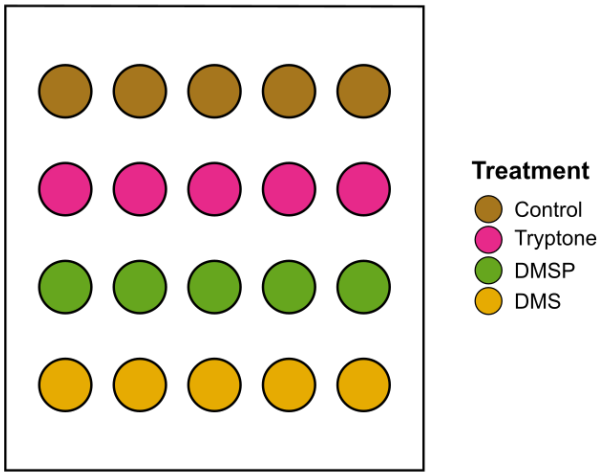

Figure S5.1: Schematic of ISCA diagram showing non-randomised distribution of treatments within each ISCA used for preliminary trials. This setup was used in high-nutrient trials, in Experiment 1.

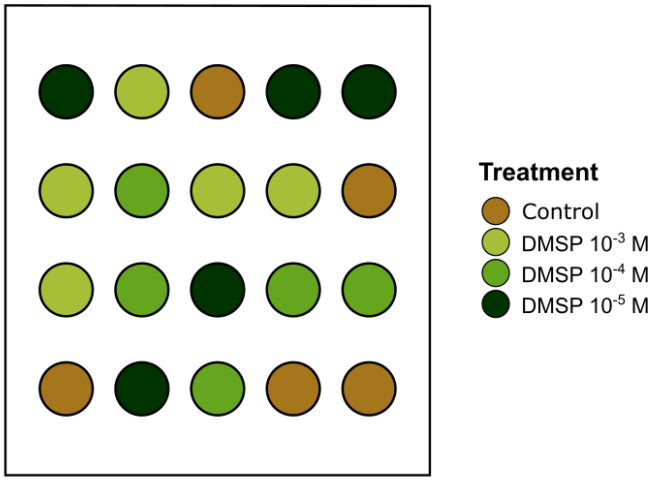

Figure S5.2: Example of ISCA chemical treatments using randomised treatments. This setup was used in low-nutrient trials, in Experiment 2.

Response of Breviolum minutum and Cladocopium C1acro to Tryptone, DMSP and DMS in high nutrient media

B. minutum and *C. C1acro* were both significantly attracted to tryptone; *B. minutum* had 2.1× more cells in the tryptone wells, and *C. C1*^{acro} had 6.24× more cells in the tryptone wells (Wilcoxon test, p <0.05 for both species; Fig. S3, Table S3). *B. minutum* and *C. C1acro* exhibited different behavioural

responses to both dimethylsulphoniopropionate (DMSP) and dimethyl sulphide (DMS; Fig. 1). Indeed, *B. minutum* was significantly repelled by DMSP and DMS (Wilcoxon test, $p < 0.005$; Table S3), with 1.9-times fewer cells in the DMSP treatment and 2.48-times fewer cells in the DMS treatment compared to negative controls. In contrast, *C. C1^{acro}* exhibited no significant response to these chemicals (Wilcoxon test, $p < 0.05$; Table S3).

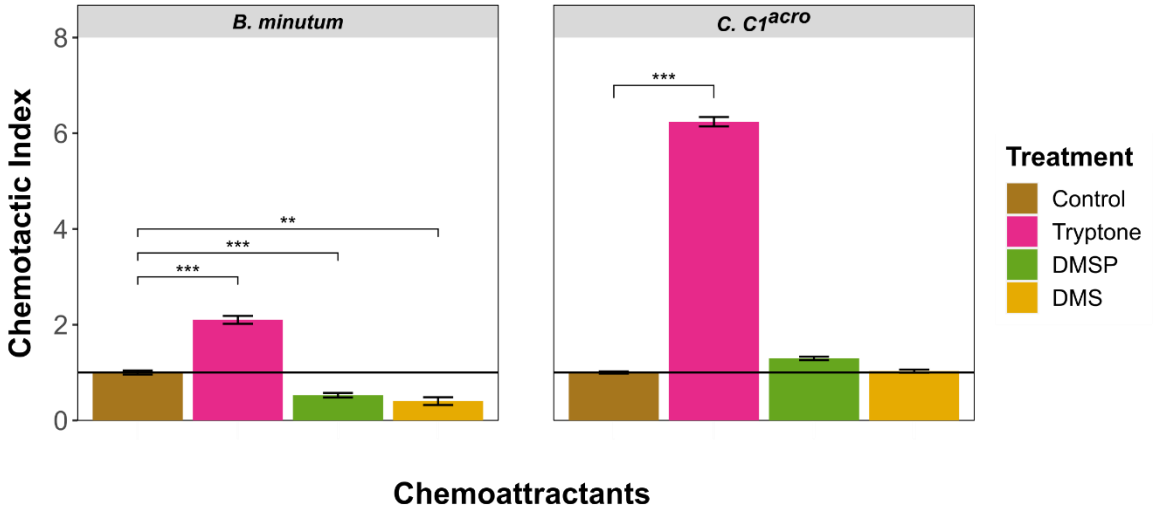

Figure S5.3: *Breviolum minutum* and *Cladocopium C1acro* chemotactic response to tryptone, DMSP and DMS in high nutrient media. Statistical significance denoted by asterisks: * <0.05; ** <0.01; *** <0.001. Values represent means +/- standard error; n = 4-28, see Table S3

Preliminary trial on the effect of nutrient levels on chemotactic response to Tryptone and DMSP in B. minutum and Cladocopium sp.

Since previous experiments were suggestive of a chemotactic response of *Cladocopium C1acro* to DMSP (Fig 1, Fig. S3), I hypothesised that a lower nutrient environment, more reflective of environmental nutrient conditions, would produce more chemotactically responsive algae. Additionally, prior studies have shown that high nitrogen levels in the surrounding medium decreased the symbionts' ability to respond chemotactically to nitrogen attractants, suggesting that the presence of nutrients suppresses chemotactic behaviour (Fitt, 1985). During Experiment 1, all chemotaxis experiments were performed in high nutrient medium; to test the effect of background nutrients on the chemotactic response of Symbiodiniaceae, an experiment was performed (Experiment 2) using two nutrient conditions (high and low) in the surrounding medium, with two species of Symbiodiniaceae (*B. minutum* and *Cladocopium* sp.). Cultured *B. minutum* and *Cladocopium* sp. were transferred to 50

mL Falcon tubes during the benthic portion of their lifecycle and centrifuged at 500 × g for 5 min. The algal growth medium was removed and replaced with sterile artificial seawater. ISCA trials were run five days later during the motile phase of their lifecycle. All subsequent chemotaxis trials (Experiment 2) were performed using this nutrient-depleted method.

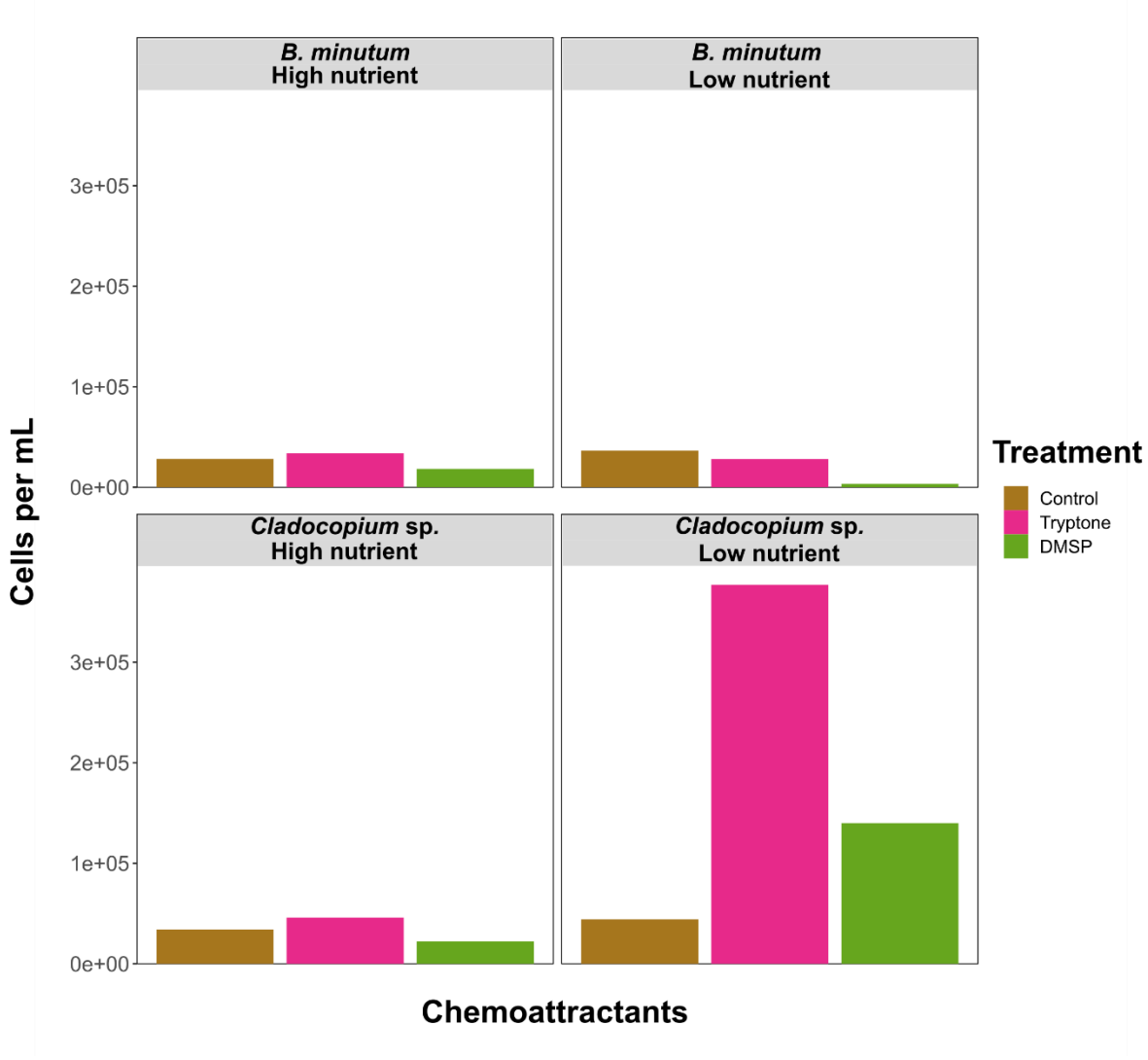

Figure S5.4: *Breviolum minutum* and *Cladocopium goreauii* response to tryptone and DMSP in high and low nutrient media. One trial only *per* data-point.

Table S5.1: Quantum yield measurements (+/- standard error) of *B. minutum*, *C. goreauii* and *D. trenchii* after incubation in low nutrient artificial seawater for 5 days (n = 5 for each species), prior to chemotaxis trials. Symbiodiniaceae were dark adapted for 15 minutes before quantum yield measurements were taken.

Species	Average quantum yield (fv/fm)	Standard error
B. minutum	0.544	0.0165
C. goreuiii	0.551	0.0205
D. trenchii	0.531	0.0097

Table S5.2: Chemotactic indices of putative chemicals for use as positive control across four species of Symbiodiniaceae: *Breviolum minutum*, *Cladocopium C1^{acro}*, *Durusdinium trenchii* and *Symbiodinium microadriaticum*. Ic = chemotactic index; SD = standard deviation; SE = standard error; n = number of biological replicates. Trials from Experiment 1.

Species	Treatment	Ic mean	Ic SE	n	Fold-change relative to control wells	*p*-value
B. minutum	Control	1	0.04	11	-	-
B. minutum	Tryptone	2.10	0.08	11	2.10	0.0004
B. minutum	DMSP	0.53	0.05	7	-1.90	0.0009
B. minutum	DMS	0.40	0.08	4	-2.48	0.005
B. minutum	BrCl2CH	0.65	0.14	4	-1.53	0.182
B. minutum	I2CH2	0.82	0.14	4	-1.22	0.316
B. minutum	Mannitol	0.78	0.17	3	-1.28	0.316
C. goreaui	Control	1	0.02	28	-	-
C. goreaui	Tryptone	6.24	0.10	20	6.24	4.8e-11
C. goreaui	DMSP	1.30	0.04	20	1.30	0.185
C. goreaui	DMS	1.03	0.03	16	1.03	0.821
C. goreaui	BrCl2CH	0.68	0.14	4	-1.47	0.209
C. goreaui	I2CH2	0.85	0.20	4	-1.18	0.696
C. goreaui	Glutamate	0.97	0.18	4	-1.03	0.821
D. trenchii	Control	1	0.16	4	-	-
D. trenchii	Tryptone	3.05	0.29	4	3.05	0.059
D. trenchii	DMSP	0.77	0.14	4	-1.30	0.552
D. trenchii	Glutamate	0.65	0.09	4	-1.55	0.368
S. microadriaticum	Control	1	0.11	4	-	-
S. microadriaticum	Tryptone	1.38	0.12	4	1.38	0.11
S. microadriaticum	DMSP	0.86	0.13	4	-1.16	0.41
S. microadriaticum	Glutamate	0.76	0.10	4	-1.13	0.17

Table S5.3: Chemotactic response to tryptone, DMSP and DMS by *B. minutum* and *C. C1*^{acro} in high nutrient media. Ic = chemotactic index; SD = standard deviation; SE = standard error; n = number of biological replicates. Experiment 1.

Species	Treatment	Ic mean	Ic SE	n	Fold-change relative to control wells	*p*-value
B. minutum	Control	1	0.04	11	-	-
B. minutum	Tryptone	2.10	0.08	11	2.10	0.0001
B. minutum	DMSP	0.53	0.05	7	-1.90	0.0005
B. minutum	DMS	0.40	0.08	4	-2.48	0.004
C. goreaui	Control	1	0.02	28	-	-
C. goreaui	Tryptone	6.24	0.10	20	6.24	1.36e-11
C. goreaui	DMSP	1.30	0.04	20	1.30	0.211
C. goreaui	DMS	1.03	0.03	16	1.03	0.781

Table S5.4: Preliminary trial testing chemotactic response of *B. minutum* and *C. goreauii* to tryptone and DMSP in two different nutrient conditions in Experiment 2.

Species	Nutrient Level	Treatment	cells/ml
B. minutum	Low	ASW	36500
B. minutum	Low	Tryptone	28100
B. minutum	Low	DMSP	3400
B. minutum	High	ASW	28200
B. minutum	High	Tryptone	33700
B. minutum	High	DMSP	18300
C. goreauii	Low	ASW	44300
C. goreauii	Low	Tryptone	377100
C. goreauii	Low	DMSP	139900
C. goreauii	High	ASW	34100
C. goreauii	High	Tryptone	45900
C. goreauii	High	DMSP	22400

Table S5.5: Chemotactic response to tryptone and DMSP by *B. minutum, C. goreauii* and *D. trenchii* in low nutrient media. Ic = chemotactic index; SD = standard deviation; SE = standard error; n = number of biological replicates in Experiment 2.

Species	Treatment	Ic mean	Ic SE	n	Fold-change relative to control	
B. minutum	Control	1	0.21	8	-	-
B. minutum	Tryptone	1.73	0.29	8	1.73	0.015
B. minutum	DMSP	0.29	0.03	8	-3.45	0.0002
C. goreauii	Control	1	0.55	4	-	-
C. goreauii	Tryptone	99.8	14.85	4	99.8	0.044

C. goreauii	DMSP	1.01	0.43	4	1.01	1.00
D. trenchii	Control	1	0.17	4	-	-
D. trenchii	Tryptone	4.64	0.33	4	4.64	0.043
D. trenchii	DMSP	0.84	0.23	4	-1.2	0.486

Table S5.6: Chemotactic response to DMSP at three different concentrations by *B. minutum* and *C. goreauii* in low nutrient media. Ic = chemotactic index; SD = standard deviation; SE = standard error; n = number of biological replicates.

Species	**Treatment**	**Ic mean**	**Ic_SE**	**n**	**Fold-change relative to control**	***p*-value**
B. minutum	Control	1	0.18	5	-	-
B. minutum	DMSP 10^{-3}	0.19	0.04	5	-5.2	0.0007
B. minutum	DMSP 10^{-4}	0.37	0.12	5	-2.7	0.0064
B. minutum	DMSP 10^{-5}	0.30	0.07	5	-3.3	0.0027
C. goreauii	Control	1	0.13	16	-	-
C. goreauii	DMSP 10^{-3}	0.77	0.14	16	-1.31	0.94
C. goreauii	DMSP 10^{-4}	1.81	0.44	16	1.81	1.00
C. goreauii	DMSP 10^{-5}	1.58	0.38	16	1.58	1.00