

Supplementary Materials

Table S1. MRM conditions for each metabolite.

Metabolite	Parent (<i>m/z</i>)	Product (<i>m/z</i>)	CV (V)	CE (V)	Polarity	Quantifier/Qualifier
DHPS	155	95	2	14	Negative	Quantifier
		80	2	30	Negative	Qualifier
DMSP	135	73	2	12	Positive	Quantifier
		63	2	12	Positive	Qualifier
		45	2	23	Positive	Qualifier

CV, cone voltage.

CE, optimized collision energies.

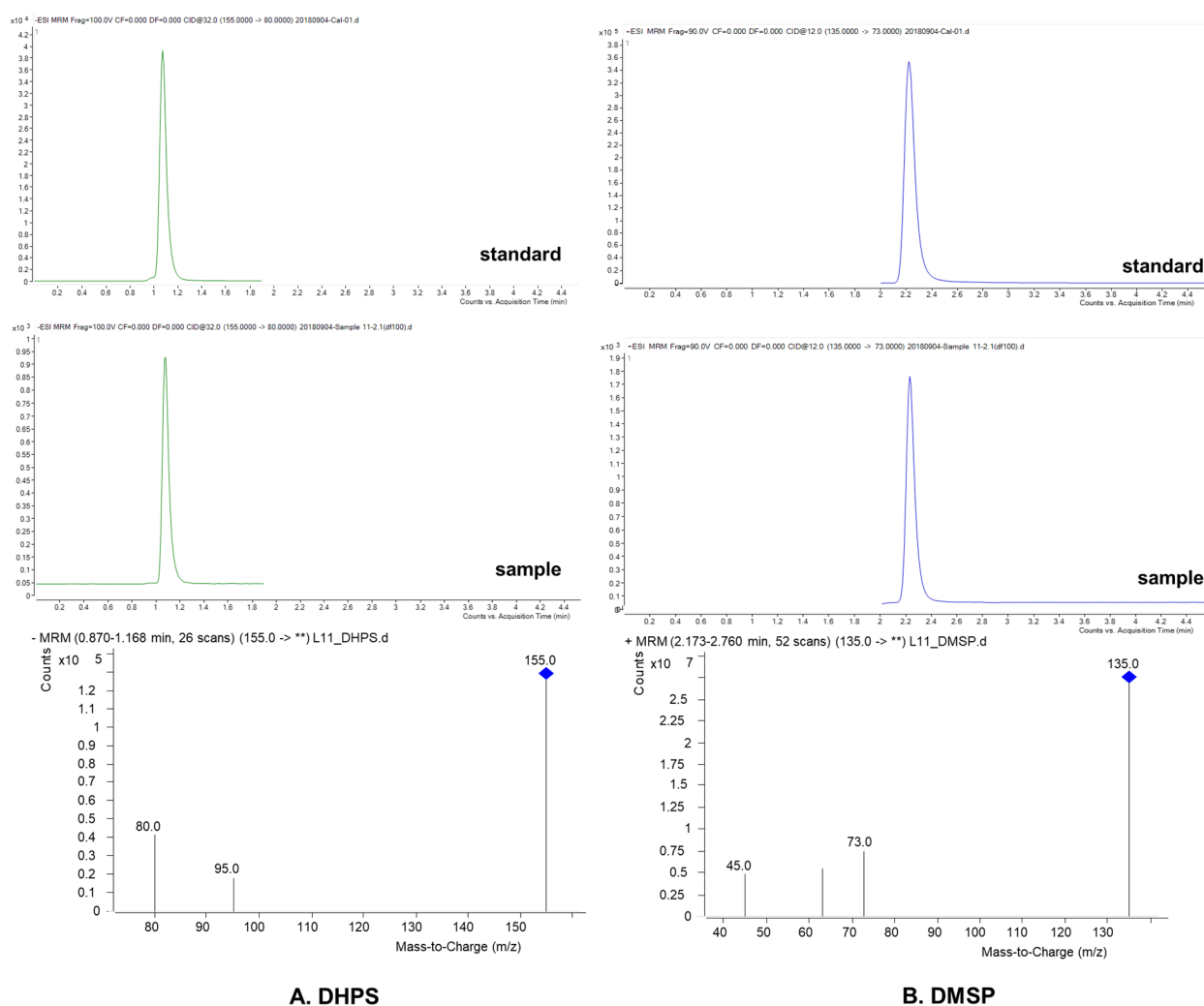


Figure S1. Analysis of DHPS (A) and DMSP (B) via targeted LC-MS/MS. The extracted ion chromatograms (EICs) from standard solutions (upper figures) and samples (middle figures) of the targeted analytes under the optimal conditions. The MS/MS characteristics of DHPS and DMSP are also shown (lower figures).

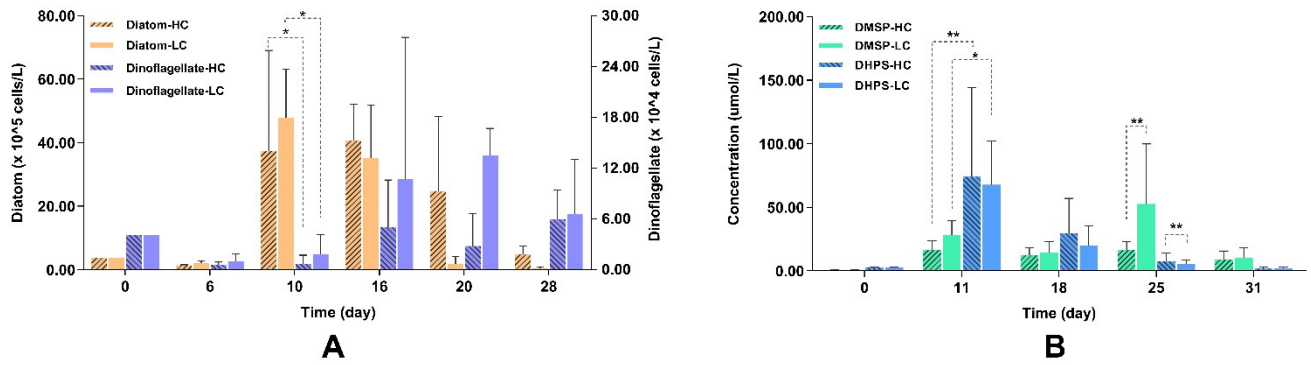


Figure S2. Community succession of the predominate phytoplankton (A), and concentrations of DHPS and DMSP (B) during the mesoscale experiment. HC: high $p\text{CO}_2$ treatment groups, 1000 ppmv; LC: low $p\text{CO}_2$ treatment groups, ~410 ppmv. (A) Data were quoted from [24]; Error bars represent standard deviation of replicates for different treatments (HC, $n = 4$; LC, $n = 3$). (B) The metabolite concentrations were present as the mean values with standard deviation of triplicate samples for replicate cultured bags ((HC, $n = 12$; LC, $n = 9$) with the same treatment. Two-way ANOVA analysis, *, $p < 0.05$; **, $p < 0.01$.