

Fig. S1 Ordination analysis of the *nifH* community structure using unweighted PCoA (A) and NMDS analysis based on Bray-Curtis distance matrix (B). A trend of separation could be found in both analyses.



Fig. S2 Response ratio analysis of significantly changed *nifH* OTUs. Relative abundance and genus assignment for these OTUs were also included. Error bars plotted at the right side of the dashed line indicate significantly increased relative abundance at eCO2, while error bars plotted at the left side indicate significantly decreased relative abundance at aCO2.



Fig. S3 All *nifH*-centered modules identified in this study. Only modules with >5 nodes were included. Diamond nodes represent nifH OTUs. Circular nodes represent 16S OTUs.