

Description of Additional Supplementary Files

Supplementary Data 1. Sample metadata of Antarctic soils.

Supplementary Data 2. Summary statistics of archaeal and bacterial MAGs assembled from Antarctic soils.

Supplementary Data 3. HGT events of 676 microbial genomes in Antarctic soils.

Supplementary Data 4. Community-level HGTs across different microbial phyla (upper), pairwise HGT frequencies between phyla (middle), and HGT frequencies normalized by the product of phylum relative abundances (lower) in Antarctic soils.

Supplementary Data 5. The association between the number of HGT events per species and their co-occurrences.

Supplementary Data 6. The phylogenetic distances between MAG pairs.

Supplementary Data 7. Functional distribution of horizontally transferred genes based on COG categories.

Supplementary Data 8. Annotation of genes representing different energy conservation and carbon acquisition pathways in 676 MAGs.

Supplementary Data 9. Annotation of MGE genes in 676 MAGs.

Supplementary Data 10. pN/pS value of hydrogenase genes across 16 Antarctic soil samples.

Supplementary Data 11. pN/pS value of aerotrophy genes in an independent set of nine Antarctic metagenomes from geographically distinct regions (Dronning Maud Land, Robinson Ridge, and Bunger Hills).

Supplementary Data 12. dN/dS results for aerotrophy genes comparing test (Antarctic) and reference (non-Antarctic) groups using RELAX, based on 50 independent subsampling replicates.

Supplementary Data 13. dN/dS results for aerotrophy genes comparing test (Antarctic) and reference (non-Antarctic) groups using RELAX, based on 50 independent subsampling replicates. $K > 1$: intensified selection strength, $K < 1$, relaxed selection strength.

Supplementary Data 14. Site-level selection results of [NiFe] group 1I hydrogenases inferred using MEME and FEL in HyPhy. Both methods are likelihood-based codon substitution models; statistical significance was assessed using likelihood ratio tests (two-sided).

Supplementary Data 15. Principal component analysis (PCA) based on pN/pS values of [NiFe] Group 1h and 1I across samples. P-values represent permutation-based significance tests (999 permutations) assessing correlations between environmental variables and principal components.

Supplementary Data 16. $pN^{(site)}$ and $pS^{(site)}$ toward RSA and DTL for hydrogenases in the complex.

Supplementary Data 17. Residue-level evolutionary conservation scores of the target hydrogenase.