**Supporting Information** 

# Deterministic assembly processes shaping habitat-specific glycoside hydrolase composition

List:

Figure S1-S13, Data S1-S4.



**Figure S1. Differences in GH abundance within prokaryotic communities in different environments.** The OTUs corresponding to the CAZy genomes were determined based on a 16S rRNA-V4 region identity of greater than 98.6% or 100%. The GH abundance was calculated separately for the two sample sets, with each grey point representing an EMP sample. For the boxplots, the middle line indicates the median, the box represents the 25th-75th percentile, and the whisker indicates the 10th-90th percentile of observations. EMPO classified 17 microbial environments (level 3) into freeliving or host-associated (level 1), and saline or non-saline (for free-living) or animal or plant (for hostassociated) (level 2). Host-associated environments are represented in cyan, while free-living environments are represented in orange.



Figure S2. Deterministic processes dominate the assembly of GH communities. Pairwise Raup-Crick between communities indicates that the GH genes are either more similar (-0.95 > Raup-Crick > -1) or less similar (0.95 < Raup-Crick < 1) to each other than expected by random chance (1000 randomizations). Any other value of Raup-Crick indicates that the GH communities are stochastically assembled (-0.95 < Raup-Crick < 0.95). The vertical dashed lines mark the positions of -0.95 and 0.95 in panels. The contribution ratios of deterministic and stochastic processes are also marked in panels.



**Figure S3. Similarity of GH composition across various environments.** Principal coordinate analysis (PCoA) of the GH distribution characteristics in EMPO level 3 environments was performed using the PAST3 software based on the Bray-Curtis method.



Figure S4. A co-occurrence network diagram exhibiting the correlations between various GH families within the environment. The EMPO classified environmental samples into 17 microbial environments. The hypersaline (saline) environmental samples were too few to be displayed. A co-occurrence network was constructed by Gephi, and the pairwise Spearman's  $\rho$  and p values were determined using the "psych" package in R. Values of Spearman's  $\rho > 0.8$  and p < 0.01 were considered to indicate valid relationships (connecting lines in the network diagram).



Figure S5. Potential impact of prokaryotic-encoded GHs on their environmental adaptability. Comparisons between bins were analyzed using the Wilcoxon rank test. \*\* p < 0.01, \*\*\* p < 0.001.



**Figure S6. Taxonomic source statistics of GH families in all EMP samples.** The number of prokaryotic genera encoding GHs in EMP samples was counted using the NCBI Taxonomy database. The different colors in the figure indicate the prokaryotic genera from distinct taxonomic groups.







**Figure S8. Most common prokaryotic genera of GH families in EMPO environments.** The most common prokaryotic genus was defined as the genus that appeared in the most samples and had an occupancy of at least 0.05 in all samples. The EMP samples were classified into 17 microbial environments by EMPO. Different colors represent different taxonomic groups. The circle size indicates the occupancy of the genus in all samples within a single environment. Only 76 GH families with an occupancy of less than 0.75 in all EMP samples are displayed, and the other 76 GH families are shown in Figure 7. Specific information on the prokaryotic genera can be found in Figure S9.

Proteobacteria	
Alphaproteobacteria	<i>a</i> . <i>i</i> .
All Al2	Spningomonas Bradyrhizobium
A13	Sphingobium
A14 A15	Celeribacter
Al6	Sulfitobacter
Al8	Brevundimonas
Al9	Caulobacter Processia
All1	Nordella
A112	Pseudolabrys Agrobactorium
A113 A114	Ensifer
Al15 Al16	Paracoccus Frythrobacter
A117	Pseudohalocynthiibacter
Al18 Al19	Ancylobacter Bartonella
Al20	Devosia
A121 A122	Rhodobacteraceae
A123	Sphingosinithalassobacter
A124 A125	Boseongicola
A126	Commensalibacter Eleviibacterium
A127 A128	Gramilihacter
Al29	Methylobacterium
A130 A131	Pelagihaca
A132 A133	Rhodovulum Sphingopyris
Al34	Beijerinckia
A135 A136	Labrenzia Mesorhizohium
A137	Rhodobacter
Al38 Betaproteobacteria	Starkeya
Bel	Mitsuaria
Be2 Be3	Janthinobacterium Acidovorax
Be4	Methylibium
Be6	Lauropia Rhodoferax
Be7	Snodgrassella
Bes Be9	Deijna Methylophihis
Bel0 Bel1	Neisseria Remohanthaldonia
Bel2	Bordetella
Bel3 Bel4	Candidatus Nitrotoga Cupriavidus
Be15	Herbaspirillum
Bel6 Bel7	Massilia Ralstonia
Be18	Alicycliphilus
Be19 Be20	Belaproteonacteria Dechloromonas
Be21	Rhizobacter
della/epsilon subdivisions del	Corallococcus
de2	Labilithrix Psaudanhvaromvya
de4	Minicystis
de5 de6	Chondromyces Desulfobacula
de7	Geobacter
de8 Gammaproteobacteria	Pelohacter
Gal	Pseudomonas
Ga2 Ga3	Raoultella
Ga4 Ga5	Acinetobacter Psaudoaltaromonae
Ga6	Cellvibrio
Ga7 Ga8	Gilliamella Xanthomonas
Ga9	Microbulbifer
Ga10 Ga11	Alteromonas Kineobactrum
Ga12	Methylocaldum
Ga13 Ga14	Haemophilus Stenotrophomonas
Ga15	Teredinibacter
Galo Gal7	Colwellia
Ga18 Ga10	Dyella Saliwiwonas
Ga20	Spiribacter
Ga21 Ga22	Thioalkalivibrio Azotobacter
Ga23	Candidatus Methylospira
Ga24 Ga25	Granulosicoccus Halomonas
Ga26	Immundisolibacter
Ga27 Ga28	1.egionetta Marichromatium
Ga29	Marinomonas Mathyloreonas
Ga30 Ga31	Salinivibrio
Ga32	Serratia Marinobacter
Oligoflexia	and another ter
011	Halobacteriovorax Proteobacteria

#### Terrabacteria group Actinobacteria Herbiconiux Acl Ac2 Streptomyces Bifidobacterium Ac3 Leifsonia Pseudarthrobacter Ac4 Ac5 Ac6 Corvnebacterium Actinomyces Curtobacterium Mycolicibacterium Ac7 Ac8 Ac9 Ac10 Micromonospora Ac11 Ac12 Celhilomonas Microbacterium Ac13 Ac14 Nocardioides Schaalia Ac15 Ac16 Ac17 Ac18 Kineococcus Tetrasphaera Brachybacterium Rothia Ac19 Ac20 Ac21 Candidatus Planktophila Nocardiopsis Rhodococcus Ac22 Ac23 Ac24 Acidothermus Brevibacterium Candidatus Aquihuna Ac25 Ac26 Geodermatophilus Marmoricola Ac27 Ac28 Pauljensenia Plantactinospora Ac29 Verrucosispora Ac30 Ac31 Arthrobacter llumatobacter Ac32 Ac33 Mycobacterium Nonomuraea oflexi Ch1 Chle Caldilinea Ch2 Chloroflexus Ch3 Roseiflexus Cyanobacteria/Melainabacteria group Cyl Synechococcus Cy2 Chondrocystis Cy3 Cy4 Cy5 Cy6 Cy7 Cy8 Cy9 Cyanobium Microcoleus Nostoc Acaryochloris Anabaena Chroococcidiopsis Leptolyngbya Cy10 Calothrix Cy11 Cy12 Oscillatoria Thermoleptolyngbya Deinococcus-Thermus Dt1 Meiothermus Firmicutes Fi1 Fi2 Streptococcus Bacillus Fi3 Clostridium Paenibacillus Lactobacillus Enterococcus Fi4 Fi5 Fi6 Fi7 Ruminococcus Cohnella Lachnospiraceae [Ruminococcus] Fi8 Fi9 Fi10 Fi11 . Herbinix Fi12 Fi13 Roseburia [Clostridium] Fi14 Anoxybacillus Ei15 Blautia Fi16 Fi17 Lactococcus [Eubacterium] Fi18 Intestinimonas Fi19 Lachnoanaerobaculum Fi20 Fi21 Paeniclostridium Staphylococcus Fi22 Desulfitobacterium Exiguobacterium Exiguobacterium Pseudobutyrivibrio Romboutsia **Fi23** Fi24 Fi25 Fi26 Selenomonas Fi27 Turicibacter Thermotogae Thermotogae Th1 Fervidobacterium Pseudothermotoga Th2 Fusobacteria Fusobacteriia Ful Fu2 Leptotrichia Fusobacterium

## **PVC** group Acidobacteria Blastocatellia Vicinamibacteria Vi1 Stenosarchaea group Nitrospirae

#### FCB group Bacteroidetes/Chlorobi group Bal Bacteroides Ba2 Paraflavitalea Flavobacterium Ba3 Pedobacter Polarihacter Flavobacteriaceae Ba4 Ba5 Ba6 Prevotella Maribacter Ba7 Ba8 Ba9 Niastella Aquimarina Chitinophaga Psychroserpens Hymenobacter Ba10 Ba11 Bal2 Ba13 Ba14 Mucilaginibacter Bal5 Bal6 Capnocytophaga Niabella Bal7 Petrimonas Ba18 Prolixibacteraceae Ba19 Ba20 Urechidicola Tenacibaculum Ba21 Flavivirga Ba22 Dokdonia Ba23 Ba24 Flavisolibacter Cellulophaga Ba25 Cyclobacterium Eyenbadeernu Formosa Cytophaga Fuzebyella Pseudobacter Ba26 Ba27 Ba28 Ba29 Wenyingzhuangia Zobellia Alistipes Ba30 Ba31 Ba32 Ba33 Bernardetia Oceanihabitans Pontibacter Sphingobacterium Ba34 Ba35 Ba36 Ba37 Chryseobacterium Ba38 Cloacibacterium Draconibacterium Ba39 Ba40 Emticicia Ba41 Filimonas Ba42 Kordia Ba43 Labilibaculum Ba44 Mariniflexile Ba45 Muriicola Ba46 Ba47 Odoribacter Tannerella Ba48 Winogradskvella Algoriphagus Arcticibacterium Gramella Ba49 Ba50 Ba51 Ba52 Ignavibacteriae Ba53 Pseudarcicella Ba54 Runella Gemmatimonadetes Gemmatimonas Gel Planctomycetes Pl1 Pl2 Pl3 Mariniblastus Roseimaritima Planctomycetes Pl4 Gemmata P15 P16 Bythopirellula Isosphaera P17 Limnoglobus Verrucomicrobia Coraliomargarita Vel Ve2 Ve3 Opitutus Verrucomicrobia Lacunisphaera Akkermansia Ve4 Ve5 Acidobacteriia Candidatus Solibacter Ad1 Ad2 Acidisarcina

Ad3 Ad4 Edaphobacter Granulicella Chloracidobacterium B11 Luteitalea

### Euryarchaeota

Halorubrum St1 St2 St3 Halorhabdu Haloarcula

Nitrospira Ni1 Nitrospira

## 10

Aquificae

Spirochaetia

Aquificae

Spl

Spirochaeta

Aq1 Thermocrinis

**Figure S9. Specific information on the most common prokaryotic genera.** Based on NCBI Taxonomy statistics, different colors represent prokaryotic genera from different taxonomic groups, and subgroups are shown in bold. The genus codes correspond to those shown in Figure 7, Figure S8, and Figure S12.



Figure S10. Environmental temperature and pH affect the occupancy and abundance of GH families in prokaryotic communities. Statistical analyses were carried out based on 2381 EMP samples with recorded temperature information and 1183 samples with recorded pH values. The EMP samples were categorized into 5 groups according to environmental temperature and pH: low temp ( $\leq 10^{\circ}$ C), moderate low temp ( $\geq 10^{\circ}$ C and  $\leq 20^{\circ}$ C), medium temp ( $\geq 20^{\circ}$ C and  $< 30^{\circ}$ C), moderate high temp ( $\geq 30^{\circ}$ C and  $< 45^{\circ}$ C), and high temp ( $\geq 45^{\circ}$ C); acidic ( $\leq 5$ ), slightly acidic ( $\geq 5$  and  $\leq 6.5$ ), neutral ( $\geq 6.5$  and < 7.5), slightly alkaline ( $\geq 7.5$  and < 9) and alkaline ( $\geq 9$ ). The occupancy of each GH family in samples within different temperature or pH groups is represented by the circle size. Colors represent the median abundance of the GH family across all EMP samples where the family was detected within the same group, with values shown as GH/1000, increasing from blue to red.

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GH4	GH73	GH14	GH118		GH4	GH	73 GHI	4 GH118	
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GH8	GH77	GH44	GH120		GH8	GH	77 GH4	4 GH120	
GH9	GH78	GH45	GH121		GH9	GH	78 GH4	5 GH121	
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GH20	GH102	GH58	GH135		GH20	GH1	02 GH5	8 GH135	
GH23	GH103	GH59	GH136		GH23	GH1	03 GH5	9 GH136	
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GH25	GH105	GH64	GH138		GH25	GH1	05 GH6	4 GH138	
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GH28 GH20	GH109	GH71	GH142		GH28 CH20	GHI	09 GH7	4 GH142	
GH30	GHU3	GH75	GH145 GH147		GH30	GHI	10 GH7	5 GH143	
GH31	GH113 GH114	GH79	GH148		GH31	GH1	14 GH7	9 GH148	
GH32	GH115	GH80	GH149		GH32	GH1	15 GH8	0 GH149	
GH33	GH117	GH81	GH150		GH33	GH1	17 GH8	I GH150	
GH35	GH125	GH82	GH151		GH35	GH1	25 GH8	2 GH151	
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GH37	GH130	GH86	GH156		GH37	GH1	30 GH8	6 GH156	
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GH39	GH140	GH89	GH158		GH39	GH1	40 GH8	9 GH158	
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**Figure S11. Diverse taxonomic sources of GH families in prokaryotic communities under different environmental temperature and pH conditions.** The EMP samples were categorized into 5 groups according to environmental temperature and pH. The colors in the figure indicate the median number of source prokaryotic genera of GH families in all EMP samples from the same environment, with increasing values from blue to red.

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**Figure S12. Most common prokaryotic genera of GH families in various environments.** The most common prokaryotic genus was defined as the genus that appeared in the most samples and had an occupancy of at least 0.05 in all samples. The EMP samples were divided into 5 groups according to environmental temperatures and pH. Different colors represent different taxonomic groups. The circle size indicates the occupancy of the genus in all samples from a single environment. Specific information on the prokaryotic genera can be found in Figure S9.



**Figure S13. Variations in the abundance of GHs encoded by prokaryotic communities across different ENVO environments.** The GH abundance is expressed as the GH/1000 value, i.e., the number of GH genes per thousand prokaryotic genes in a sample. Each grey point represents an EMP sample. For the boxplots, the middle line indicates the median, the box represents the 25th-75th percentile, and the whisker indicates the 10th-90th percentile of observations.

Data S1. Data on GH abundance in EMP samples.

Data S2. Abundance of 152 GH families in EMP samples.

## Data S3. Correlations of different GH families in various environments.

Data S4. Information on taxonomic sources of GH families in prokaryotic communities.