nature microbiology

Article

https://doi.org/10.1038/s41564-023-01573-x

Environmental stress mediates groundwater microbial community assembly

Supplementary Discussion A

Some caveats should be noted. First, we need to clarify that although microbial dispersal is discussed as a stochastic process in this study, dispersal can be either deterministic or stochastic[1]. Unlike selection or drift, dispersal cannot be unambiguously treated as deterministic or stochastic[2,3]. For instance, if dispersal rates are dependent on population size, dispersal is stochastic and high-abundance species have a greater probability for dispersal than low-abundance species. However, in some cases, dispersal could have quite different rates among different species, depending on species traits and active status (e.g., spores, dormancy), which is thus deterministic. In addition, environmental conditions in a new habitat will have dramatic effects on successful species establishment, which can be species-specific and thus deterministic. Therefore, theoretically, dispersal limitation alone could not be used as a sole evidence for stochastic processes[4] because dispersal can be either deterministic or stochastic. However, in practice, many common studies still treat dispersal as neutral due to the difficulty in studying dispersal in fields in terms of dispersal trait identification, linking dispersal traits to emergent patterns of community structure, and dispersal assessment[3]. Although some microorganisms can propel themselves to a certain degree within a short distance, microbial dispersal is typically considered passive. Since passive dispersal is mostly stochastic with respect to species identity[2], microbial dispersal can be largely considered as stochastic[5].

Second, this study focused on the planktonic fractions of bacterial communities in the groundwater but did not analyze the communities in the subsurface biofilms. Microorganisms in the biofilms played important roles in the subsurface biogeochemistry, where dispersal limitation could be even more important, and selection could be more varied under heterogeneous stresses in complex structures of sediments.

In addition, all statistical approaches have defects in quantifying community assembly processes as previously discussed[1,6,7]. Some basic assumptions underlying each approach are possible to be violated, e.g., different populations within the same phylogenetic bin can be dominated by different processes, and environmental noise can lead to stochastic patterns under deterministic assembly. Thus, the estimated absolute values can be considerably different from ‘true’ values; however, the trends of relative comparisons can be meaningful[1], particularly when they are consistent among results from various complementary approaches.

Supplementary Discussion B

Selection under environmental stresses

Theoretically, higher stress will lead to greater heterogeneous selection if the stresses are heterogeneous (**Schema B**, Fig. 1b). Our results support this hypothesis: heterogeneous selection increased with stress as the second dominant process, but homogeneous selection played a small role. These results are in agreement with the observed extremely high heterogeneity of the site hydrology, geochemistry, and environmental stressors. The high heterogeneous selection was primarily due to abnormal pH, deficiency of some metal microelements, and high levels of toxic contaminants.

As major sources of stress, many heavy metals showed significant correlations with heterogeneous selection, as expected in this metal-contaminated site. Besides, pH rather than metals showed the strongest association with selection. Correspondingly, our previous study on this site found pH as the most predictable geochemical feature by the model of bacterial DNA[8]. Many other studies on soils also showed pH significantly correlated with the diversity, structure, and assembly mechanisms of microbial communities[9,10]. In metal-contaminated sites, pH could be even more important, given its obvious effect on the geochemical processes of metals[11,12] in addition to its own filtering effects on microbes. Besides, available Co and Mo in supernatant and suspended solid showed much stronger associations with heterogeneous selection than most metals. Mo is required by many key enzymes in carbon, nitrogen, and sulfur metabolisms, such as formate dehydrogenase, xanthine dehydrogenase, nitrogenase, nitrate reductase, and sulfite oxidase[13]. Mo was found as an important determinant of N cycling in farmlands[14], forests[15], moss[16], and lakes[17]. Recently, we discovered a strong negative correlation between Mo and nitrate in the ORR site and demonstrated Mo-dependent denitrification of a typical isolate from the site[18]. In this study, Mo was 0.14 ± 0.42 µM (mean ± standard deviation, n=91) in groundwater. Thus, Mo depletion induced by Fe/Al in the acidic environment was proposed as an important constraint of N cycling in this site[18]. Co serves as a component of vitamin B12 and an essential enzyme cofactor in most bacteria[19,20]. In our study, Co was 0.64 ± 2.6 µM in groundwater and not detectable in 76% wells. Even the maximum concentration (0.021 mM in a highly contaminated well) was much lower than the common toxic level for microorganisms[20,21]. On the contrary, major contaminants, e.g. nitrate, U, Cd, Al, showed concentrations up to 159-1445 folds of reference levels in contaminated areas. Their associations with heterogeneous selection were also significant (R^2_{CV} 0.030-0.073, OPLS VIP 1.2-1.7) but relatively weaker than Co and Mo (R^2_{CV} 0.074-0.122, OPLS VIP 2.1-2.3). Altogether, abnormal pH, deficiency of some metal microelements, and high level of toxic contaminants imposed obvious selective pressure on the groundwater bacterial communities.

In addition, our hypothesis is also supported by various animal and plant community studies showing an increased role of habitat filtering under higher stress[22-25]. However, the effects of multiple stressors may diminish one another (i.e., antagonistic interaction among stressors) when they are not highly stressful[26], which is possible because the responses induced by a stressor, e.g., antioxidant defense[27], extracellular polymeric substance[28], efflux pumps[29], and etc., could enhance organisms' resistance to other stressor(s). Thus, the roles of selection may increase slowly or even decrease under moderate levels of complex stresses. Besides, if the influence of heterogeneous and homogeneous selection are similarly strong, their opposite effects on β-diversity patterns may cancel out each other in null model analysis, resulting in underestimation of selection even in stressful environments[30].

Supplementary Discussion C

Dispersal limitation under environmental stresses

As opposed to selection, we predicted that dispersal limitation would increase with stress (**Schema C**, Fig. 1c) but we found a reverse trend in the experimental data (Fig. 3e). The previous prediction (Schema C) considers higher stress generally retards microbial colonization and establishment. However, in some cases, microbial dispersal does not depend on colonization but more relies on physical transport conditions, such as spatial distance, connectivity, and fluid flow[31,32]. Intuitively, microorganisms and stressors (e.g., toxic pollutants) can reach more easily to the locations with shorter distances, better connectivity, and higher flow rates, while the isolated or distant locations are less threatened by the stressors due to more limited dispersal. Consequently, the dispersal limitation can be negatively related to stress, as in this study, the lower dispersal limitation at high-stress areas corresponded to higher groundwater flow rates along the contaminants flux pathway[33]. This could be possible or even common for free-living microorganisms in contaminated surface water, groundwater, and atmosphere. Although decreased with stress, dispersal limitation played a predominant role in bacterial assembly across all stress levels, as demonstrated by several recent studies[34-36]. However, dispersal limitation did not show significant associations with coarse level geographic factors (e.g., distance, depth, screen length, elevation), and only had relatively weak associations with some chemical properties. In contrast, the map of dispersal limitation can be partly explained by some inferred geo-hydrological features (e.g., the boundaries implied by DO). These results demonstrate the necessity to develop microbial dispersal model(s) to account for complex geo-hydrological conditions rather than just simple correlations.

Supplementary Discussion D

Harnessing community assembly mechanism research for better modelling

Understanding the rules and drivers of microbial assembly under stress can also be helpful in modelling and prediction of microbial dynamics and functioning. Modelling across the scales from genes/species to ecosystems is desired for bridging basic and translational science for microbial ecology, however, is challenging due to diverse information with numerous dimensions[37]. The community assembly analysis can identify key environmental/microbial variables and essential relationships to support model construction, initiation, and calibration. Taking our study as an example, the substantial contribution of selection, dispersal limitation, and 'drift' points out the direction for model construction, i.e., integrating biogeochemistry and geo-hydrology with microbial dispersal model and stochastic null models. But the system could be too complex to integrate, considering hundreds of environmental factors and tens of thousands of taxa. A critical challenge is to simplify the model(s) with key variables. The major driving factors of microbial assembly can be key environmental variables (e.g., pH and Mo in our study site). The major taxa groups governed by selection can serve as candidate indicators in biogeochemical models. Interestingly, selection-controlled taxa in our study were mainly unclassified and as-yet uncultivated bacteria, suggesting valuable opportunities for isolation or metagenomic research to capture novel species with essential functions[38-40]. The relevant functional genes in these as-yet uncultivated taxa can be indicators for key biogeochemical processes. Besides deterministic processes, another challenge is to model microbial dispersal, which is different from the transportation of chemicals or particles and hard to track by experiments using physical/chemical tracers. To tackle the problem, assembly mechanism analysis (like iCAMP) can identify the taxa mainly controlled by dispersal, which can serve as indicators to calibrate the microbial dispersal model. In addition, the strong association between stress and some assembly processes can provide basic constraints of microbial groups governed by those processes, to set useful boundary conditions in model initiation and optimization. Besides, we want to emphasize that the key variables and specific relationships identified in one site may not be applicable to other sites, however, some general rules (as our theoretical framework is targeting) will emerge under the development of modelling integrated with assembly mechanism research.

Supplementary Notes

In this study, we proposed three different stress metrics, including maximum stress index (MSI), stressor number, and suppressed ratio of reference taxa richness (SRTR). Then, we tested four complementary options to group samples into different stress levels, including Option A based on MSI, Option B based on stressor number, Option C based on SRTR, and Option D by hierarchical clustering.

Stress metrics

(1) Maximum Stress Index (MSI)

The high concentrations of metals, H^+, OH^-, some anions, and conductivity can impose or reflect higher stress, so-called stress indicators (listed in Supplementary Table 2). For each stress indicator, Stress Index (SI) is defined as

$$SI_{ik} = \frac{C_{ik}}{Ref_i}$$

SI_{ik}	Stress index value of stress indicator *i* (e.g., uranium) in sample *k*.
C_{ik}	Observed value of stress indicator *i* (e.g., Uranium concentration) in sample *k*.
Ref_i	Reference level of stress indicator *i* (e.g., 0.03 mg/L for Uranium). The reference levels were from water quality standards or toxicity database (Supplementary Table 2).

Similar to Liebig's law, the stress level of a sample should be more determined by the stress indicator showing the maximum value of stress index. Thus, maximum stress index (MSI) is proposed as a stress metrics.

$$MSI_k = \max_i\{SI_{ik}\}$$

MSI_k	Maximum stress index value in sample *k*.

(2) Stressor Number

A stress indicator can become a stressor if its value exceeds a certain threshold. In this study, a stressor is defined as a stress indicator with stress index value higher than 1, i.e., its observed value is higher than the reference level.

$$STN_k = \sum_i \delta_{ik}$$

$$\delta_{ik} = \begin{cases} 1 & C_{ik} > Ref_i \\ 0 & C_{ik} \leq Ref_i \end{cases}$$

SN_k Stressor number in sample *k*.

δ_{ik} Operator, whether stress indicator i is counted as a stressor in sample *k*.

(3) Suppressed rate of Reference Taxa Richness (SRTR)

An environment with higher stress can generally suppress the diversity of common species that live well in an environment without obvious stress. We defined reference taxa as the taxa with mean relative abundance > 0.1% and occurrence frequency > 50% in ‘uncontaminated’ samples where no stress indicator showed a higher concentration than the reference level. The suppressed rate of reference taxa richness (SRTR) is defined as

$$SRTR_k = \frac{MRTR - RTR_k}{MRTR}$$

$$MRTR = \max_{m}\{RTR_m\}$$

$SRTR_k$ Suppressed rate of reference taxa richness in sample *k*.

$MRTR$ Maximum reference taxa richness in uncontaminated samples.

RTR_k Reference taxa richness, i.e., observed number of reference taxa, in sample *k*.

RTR_m Reference taxa richness in an uncontaminated sample m.

Grouping samples into different stress levels

(1) Option A based on MSI

We ranked the samples by MSI. Considering similar sample size at each stress level is better for statistical analysis, we assigned each group of 13 samples that are consecutive in the MSI rank, into the same stress level. Thus, the 91 samples were grouped into 7 stress levels, A1 to A7 (Supplementary Table 3 and option A in Supplementary Fig. 1). The MSI values were significantly (*P*<0.05) different between each two stress levels (Supplementary Fig. 1a).

(2) Option B based on stressor number

Stressor numbers are integers. In the presented study, the sample number of each stress number was as below.

Stressor number	0	1	2	3	4	5	6	7	9	11	12	14	15
Sample number	21	27	12	9	3	4	1	3	2	3	3	2	1

Then, it is impossible to obtain the same sample number in each group. We set following criteria for grouping: enough group number (≥ 6 groups) and each group have enough samples (≥ 8) to provide adequate statistical power; samples with the same stress number should be in the same group; stressor number values should be significantly different between each two groups (Supplementary Fig. 1f). Then, only the following grouping meets the requirements.

Stress level	B1	B2	B3	B4	B5	B6
Stressor number	0	1	2	3, 4	5 ~ 9	>9
Sample number	21	27	12	12	10	9

(3) Option C based on SRTR

Since richness values are integers, it is also difficult to adopt the simple strategy as Option A. Thus, we set similar criteria as Option B: enough group number (≥ 6 groups) and each group have enough samples (≥ 8) to provide adequate statistical power; samples with the same SRTR value should be in the same group; SRTR values should be significantly different between any two groups (Supplementary Fig. 1k). Then, the following grouping meets the requirements and give the most similar sample numbers among different groups.

Stress level	C1	C2	C3	C4	C5	C6	C7
SRTR	0~0.07	0.09~0.14	0.16~0.21	0.23~0.27	0.29~0.40	0.41~0.51	0.53~0.83
Sample number	14	13	11	15	13	12	13

(4) Option D based on hierarchical clustering

All the above options led to significant difference of ‘environmental dispersion’ between some stress levels. But, it is less clear whether the trend along stress levels was caused by stress increase or the changes of environmental heterogeneity. Besides, other options did not simultaneously count in all stress indicators when assessing difference among samples. Thus, we applied Option D to group the samples. First, samples were subjected to hierarchical clustering based on the concentrations of all stress indicators. Then, the following criteria were set to search for optimum grouping: samples in the same group should be clustered closer than with any sample from other groups; environmental dispersion evaluated by permutational test of multivariate homogeneity of groups dispersions (PERMDISP)[41] should have no significant difference between any two groups; enough group number (≥ 5 groups) and each group have enough samples (≥ 8) to provide adequate statistical power; stress metrics values should be generally different among groups.

As the grouping was based on the hierarchical clustering results, when group number was 6 or more, there was always at least one cluster had too few samples (<8). When separating the samples into 5 clusters, we can obtain a minimum of 8 samples in a cluster. Then, we randomly draw 8 samples from each cluster to get 5 groups of samples and test their difference in environmental dispersion; we kept trying until the obtained 5 groups showed no significant difference in environmental dispersion. In this way, we finally achieved an equal dispersion grouping of 40 samples (8 samples per group × 5 groups).

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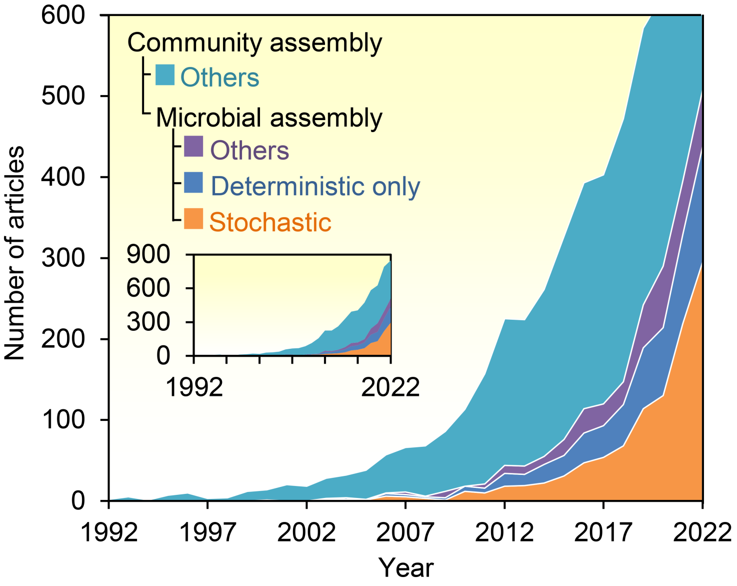
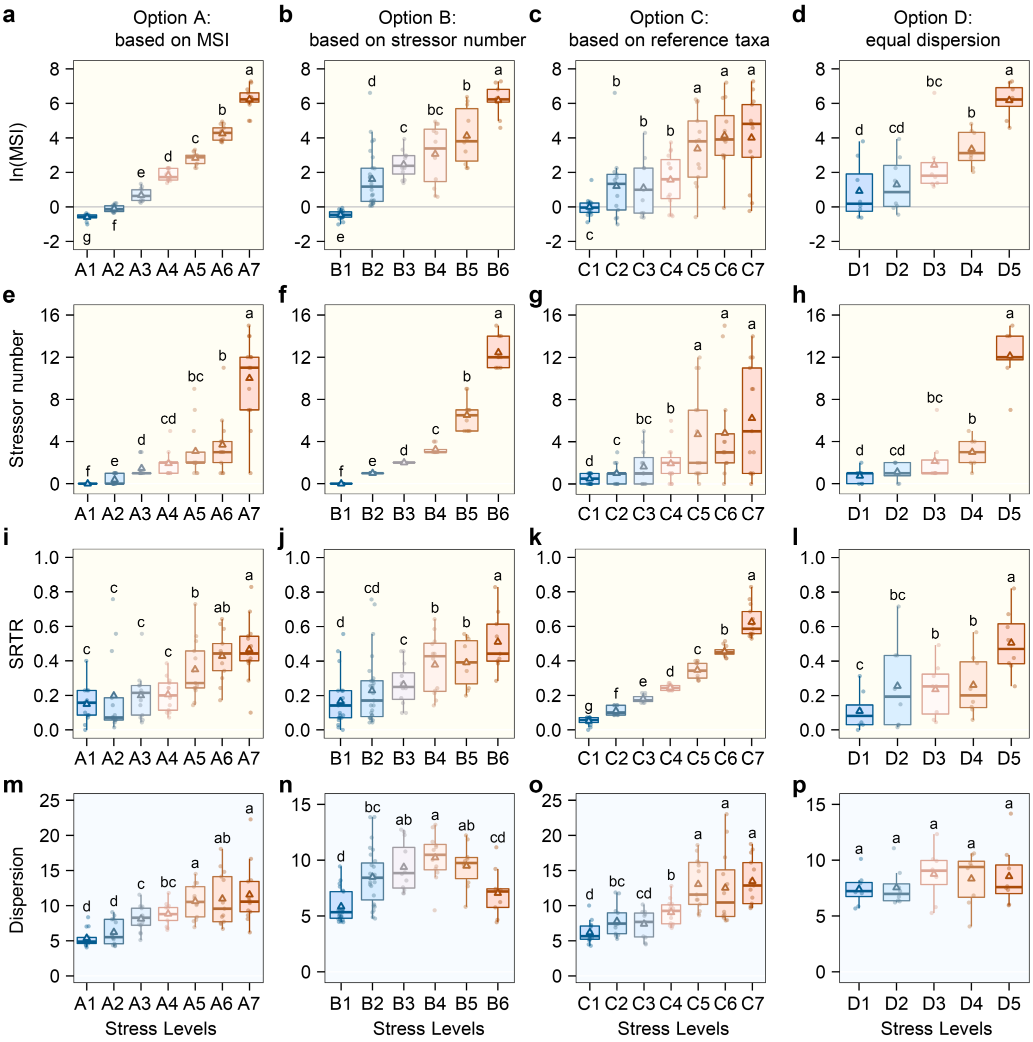
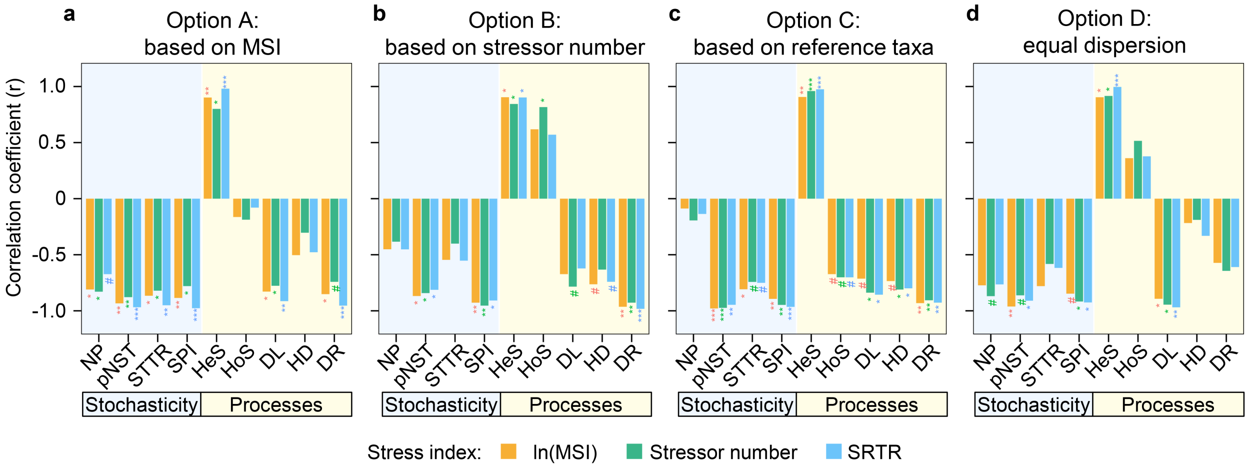


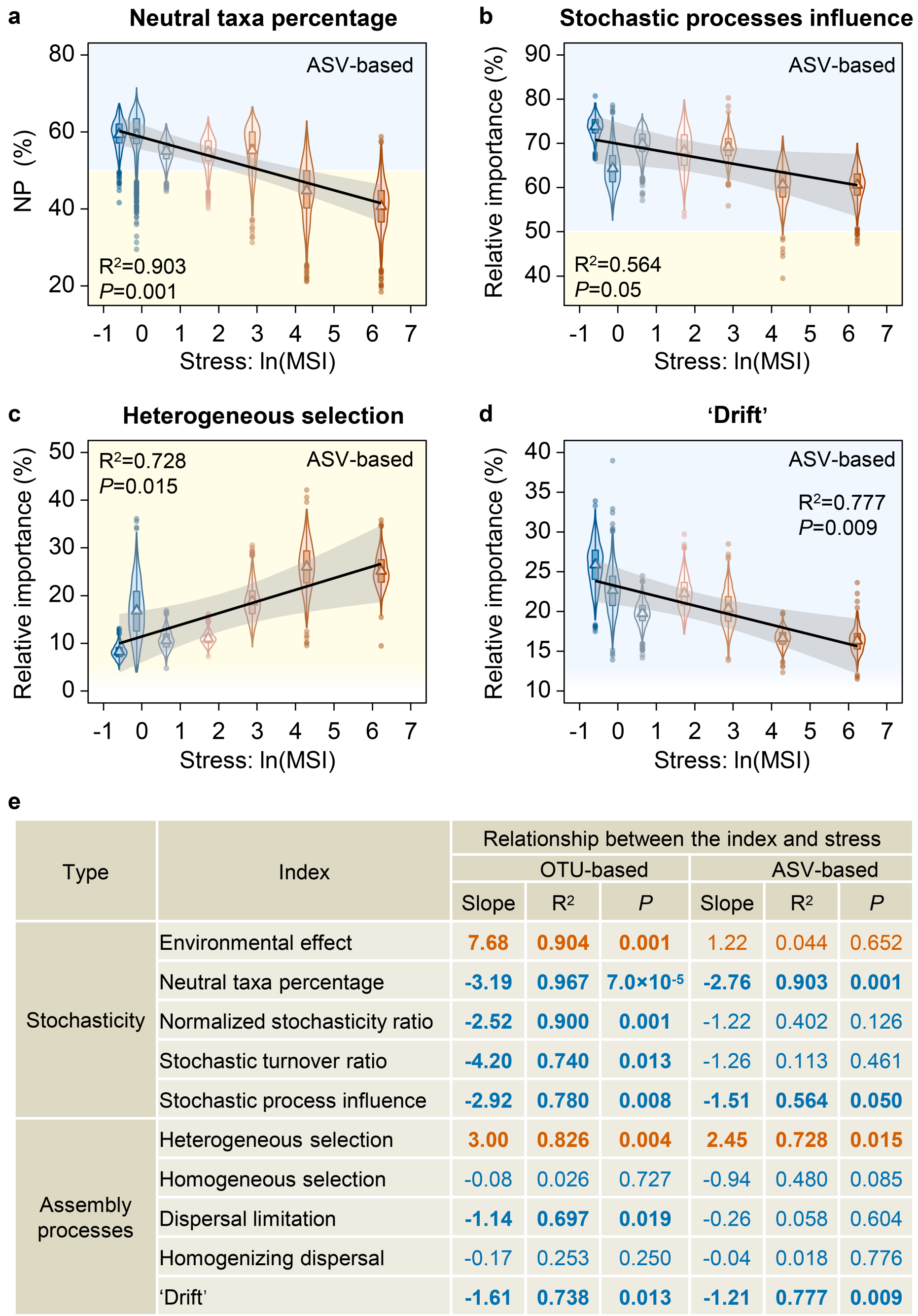
Supplementary Fig. 1. Trends in studying community assembly mechanisms. This figure is modified from Figure 1 in our previous publication (Zhou and Ning, 2017, doi:10.1128/mmbr.00002-17). The data shown are based on the annual number of articles on community assembly (any organisms, including microorganisms [inset]), articles on microbial community assembly, articles about only deterministic microbial assembly, and articles involving stochastic microbial assembly. We searched articles from 1990 to 2022 in the Web of Science Core Collection database on April 4th, 2023. To find articles on "community assembly," we searched by topic = "community assembly" and Indexes = SCI-EXPANDED and ESCI. To find articles on "microbial assembly," we searched by topic = (microbi* or bacteri* or fungi or fungus or fungal or archaea* or protist or metazoa* or mycorrhiza) in addition to "community assembly." For articles on "stochastic," we searched by topic = (neutral or stochast* or dispersal or migration or immigration or (priority effect) or (historical contingency) or drift or diversification or speciation) in articles on "microbial assembly." For articles on "deterministic only," we searched by topic = (niche or deterministic or selection or filtering or competiti* or facilitati* or mutualism or predation or interaction) in articles on "microbial assembly," except for those related to "stochastic." In 2022, around **60%** "community assembly" articles were related to "microbial assembly".



Supplementary Fig. 2. Assessment of stress and environmental dispersion at each stress level defined by different grouping options. a-d, natural logarithm of maximum stress index (MSI) at each stress level; **e-h**, stressor number at each stress level; **i-l**, suppressed rate of reference taxa richness (SRTR) at each stress level; **m-p**, environmental dispersion at each stress level. The samples were grouped into different stress levels based on MSI (option A: panels a, e, i, m), stressor number (option B: panels b, f, j, n), or SRTR (option C: panels c, g, k, o), or by hierarchical clustering and selected to make different groups show similar environmental dispersion (option D: panels d, h, l, p). Sample size in option A: n=13 in each level; option B: n=21, 27, 12, 12, 10, and 9 in Levels B1 to B6, respectively; option C: n=14, 13, 11, 15,13, 12, and 13 in Levels C1 to C7, respectively; option D: n=8 in each level. The 'reference taxa' are defined as relatively abundant and common taxa in uncontaminated samples. The 'environmental dispersion' is calculated as multivariate dispersions based on Euclidean distances of standardized geochemical properties among samples within each stress level. Colors of box plots represent the stress levels. In box plots, center line, median; box limits, upper and lower quartiles; whiskers, 1.5x interquartile range; dots, outliers; triangle, mean value at each stress level; different letters above boxes indicate significant difference among stress levels ($P<0.05$). The P values (one-sided) were calculated based on 1000-time bootstrapping test of mean value differences in panels a-l and permutational test of multivariate homogeneity of groups dispersions (PERMDISP) in panels m-p. The calculated P values are listed in the Supplementary Data file for this figure.



Supplementary Fig. 3. Correlation of stochasticity or assembly processes with different stress metrics under different grouping options. The samples were grouped to different stress levels based on (**a**) maximum stress index (MSI), (**b**) stressor number, (**c**) reference taxa richness, or (**d**) grouped to equal dispersion after hierarchical clustering. X-axis shows indexes for assessing stochasticity or influence of different assembly processes. NP, neutral taxa percentage weighted by relative abundance; pNST, normalized stochasticity based on phylogenetic null model; STTR, stochastic turnover rate estimated with entire-community null model framework QPEN; SPI, stochastic process influence estimated with phylogenetic-bin-based null model framework iCAMP; HeS, heterogeneous selection; HoS, homogeneous selection; DL, dispersal limitation; HD, homogenizing dispersal; DR, ‘drift’. Bar colors indicate different indexes for stress assessment; orange, natural logarithm of MSI; green, stressor number; blue, suppressed rate of reference taxa richness (SRTR). #, *P*<0.1; *, *P*<0.05; **, *P*<0.01; ***, *P*<0.001; the *P* values (two-sided) are based on Pearson correlation test. The calculated *P* values are listed in the Supplementary Data file for this figure.



Type	Index	Relationship between the index and stress					
		OTU-based			ASV-based		
		Slope	R^2	*P*	Slope	R^2	*P*
Stochasticity	Environmental effect	**7.68**	**0.904**	**0.001**	1.22	0.044	0.652
	Neutral taxa percentage	**-3.19**	**0.967**	**7.0×10^{-5}**	**-2.76**	**0.903**	**0.001**
	Normalized stochasticity ratio	**-2.52**	**0.900**	**0.001**	-1.22	0.402	0.126
	Stochastic turnover ratio	**-4.20**	**0.740**	**0.013**	-1.26	0.113	0.461
	Stochastic process influence	**-2.92**	**0.780**	**0.008**	**-1.51**	**0.564**	**0.050**
Assembly processes	Heterogeneous selection	**3.00**	**0.826**	**0.004**	**2.45**	**0.728**	**0.015**
	Homogeneous selection	-0.08	0.026	0.727	-0.94	0.480	0.085
	Dispersal limitation	**-1.14**	**0.697**	**0.019**	-0.26	0.058	0.604
	Homogenizing dispersal	-0.17	0.253	0.250	-0.04	0.018	0.776
	'Drift'	**-1.61**	**0.738**	**0.013**	**-1.21**	**0.777**	**0.009**

Supplementary Fig. 4. Relationship between stress and stochasticity or assembly processes estimated from amplicon sequence variant (ASV) results. **a**, Abundance-weighted neutral taxa percentage; **b**, Relative importance of stochastic processes; **c**, Heterogeneous selection; **d**, 'Drift' along stress gradient represented by log-transformed maximum stress index (MSI). **e**, Comparison between OTU-based and ASV-based results on the relationship between log-transformed MSI and stochasticity or assembly processes. OTUs and ASVs were identified using UPARSE and UNOISE, respectively. In panel **a** to **d**, the violin and box plots are based on bootstrapping results at each stress level (n=13 in each level; bootstrapping 1000 times); colors of violin plots indicate the stress levels. In box plots, center line, median; box limits, upper and lower quartiles; whiskers, 1.5x interquartile range; dots, outliers; triangle, mean value at each stress level. Black line, gray shadow, R^2, and *P* are the trendline, 95% confidence interval, coefficient of determination, and significance based on linear regression of the mean values as a function of log-transformed MSI. In panel **e**, the values outside and in the parentheses indicate slope and coefficient of determination (R^2), respectively; red numbers, increase with stress; blue numbers, decrease with stress; bold numbers, significant correlation (P<0.05); P values were calculated based on linear regression of the mean values as a function of log-transformed MSI.

Supplementary Table 1 Measured environmental variables.

No.	Variable name	Type	Notes
1	Coordinate-Eastward	Geographic factor	The coordinates were transformed to geographic distance before further analysis.
2	Coordinate-Northward	Geographic factor	
3	Elevation	Geographic factor	
4	Depth (T)	Geographic factor	The depth of the top of screen or open interval of each well
5	Depth (B)	Geographic factor	The depth of the bottom of screen or open interval of each well
6	Screen	Geographic factor	The screen or open interval size
7	Temperature or Temp	Temperature	
8	Redox	Redox-related	Redox potential
9	DO	Redox-related	Dissolved oxygen
10	DIC	Carbon-related	Dissolved inorganic carbon
11	DOC	Carbon-related	Dissolved organic carbon
12	O_2	Gas	Dissolved Oxygen concentration measured by GC
13	CH_4	Gas	Dissolved Methane concentration measured by GC
14	CO_2	Gas	Dissolved Carbon dioxide concentration measured by GC
15	N_2	Gas	Dissolved Nitrogen concentration measured by GC
16	N_2O	Gas	Dissolved Nitrous oxide concentration measured by GC
17	pH	ion (pH)	
18	Conductivity or Cond	ion	
19	Sulfide	ion	
20	Cl	ion	Chloride, anion concentration
21	Br	ion	Bromide, anion concentration
22	NO_3	ion	Nitrate, anion concentration
23	NO_2	ion	Nitrite concentration in supernatant
24	PO_4	ion	Phosphate, anion concentration
25	SO_4	ion	Sulfate, anion concentration
26	Fe(II)	Metal	Ferrous iron concentration measured in situ
27	K	Metal	
28	Na	Metal	
29	Ca	Metal	
30	Mg	Metal	
31	Al	Metal	
32	Ba	Metal	
33	Ag	Metal	
34	As	Metal	
35	Be	Metal	
36	Bi	Metal	
37	Cd	Metal	
38	Co	Metal	
39	Cr	Metal	
40	Cs	Metal	
41	Cu	Metal	
42	Zn	Metal	
43	Fe	Metal	
44	Ga	Metal	
45	Mn	Metal	
46	Li	Metal	

No.	Variable name	Type	Notes
47	Ni	Metal	
48	Pb	Metal	
49	Se	Metal	
50	Sr	Metal	
51	U	Metal	
52	U-sup	Metal in supernatant	
53	Ti-sup	Metal in supernatant	
54	V-sup	Metal in supernatant	
55	^{52}Cr-sup	Metal in supernatant	
56	^{53}Cr-sup	Metal in supernatant	
57	Mn-sup	Metal in supernatant	
58	Fe-sup	Metal in supernatant	
59	Co-sup	Metal in supernatant	
60	Ni-sup	Metal in supernatant	
61	Cu-sup	Metal in supernatant	
62	^{66}Zn-sup	Metal in supernatant	
63	^{68}Zn-sup	Metal in supernatant	
64	Ga-sup	Metal in supernatant	
65	Ge-sup	Metal in supernatant	
66	As-sup	Metal in supernatant	
67	Rb-sup	Metal in supernatant	
68	Sr-sup	Metal in supernatant	
69	^{95}Mo-sup	Metal in supernatant	
70	^{98}Mo-sup	Metal in supernatant	
71	Ru-sup	Metal in supernatant	
72	Rh-sup	Metal in supernatant	
73	Pd-sup	Metal in supernatant	
74	^{106}Cd-sup	Metal in supernatant	
75	^{111}Cd-sup	Metal in supernatant	
76	^{120}Sn-sup	Metal in supernatant	
77	Sb-sup	Metal in supernatant	
78	Te-sup	Metal in supernatant	
79	Cs-sup	Metal in supernatant	
80	Ba-sup	Metal in supernatant	
81	La-sup	Metal in supernatant	
82	Ce-sup	Metal in supernatant	
83	Pr-sup	Metal in supernatant	
84	Nd-sup	Metal in supernatant	
85	Sm-sup	Metal in supernatant	
86	Eu-sup	Metal in supernatant	
87	Gd-sup	Metal in supernatant	
88	Dy-sup	Metal in supernatant	
89	Ho-sup	Metal in supernatant	
90	Er-sup	Metal in supernatant	
91	Tm-sup	Metal in supernatant	
92	Yb-sup	Metal in supernatant	
93	Lu-sup	Metal in supernatant	
94	Hf-sup	Metal in supernatant	
95	Ta-sup	Metal in supernatant	
96	W-sup	Metal in supernatant	
97	Re-sup	Metal in supernatant	
98	Pt-sup	Metal in supernatant	
99	Tl-sup	Metal in supernatant	
100	^{208}Pb-sup	Metal in supernatant	
101	Th-sup	Metal in supernatant	
102	U-ss	Metal in suspended solid	
103	Ti-ss	Metal in suspended solid	

No.	Variable name	Type	Notes
104	V-ss	Metal in suspended solid	
105	^{52}Cr-ss	Metal in suspended solid	
106	^{53}Cr-ss	Metal in suspended solid	
107	Mn-ss	Metal in suspended solid	
108	Fe-ss	Metal in suspended solid	
109	Co-ss	Metal in suspended solid	
110	Ni-ss	Metal in suspended solid	
111	Cu-ss	Metal in suspended solid	
112	^{66}Zn-ss	Metal in suspended solid	
113	^{68}Zn-ss	Metal in suspended solid	
114	Ga-ss	Metal in suspended solid	
115	Ge-ss	Metal in suspended solid	
116	As-ss	Metal in suspended solid	
117	Rb-ss	Metal in suspended solid	
118	Sr-ss	Metal in suspended solid	
119	^{95}Mo-ss	Metal in suspended solid	
120	^{98}Mo-ss	Metal in suspended solid	
121	Ru-ss	Metal in suspended solid	
122	Rh-ss	Metal in suspended solid	
123	Pd-ss	Metal in suspended solid	
124	^{106}Cd-ss	Metal in suspended solid	
125	^{111}Cd-ss	Metal in suspended solid	
126	^{120}Sn-ss	Metal in suspended solid	
127	Sb-ss	Metal in suspended solid	
128	Te-ss	Metal in suspended solid	
129	Cs-ss	Metal in suspended solid	
130	Ba-ss	Metal in suspended solid	
131	La-ss	Metal in suspended solid	
132	Ce-ss	Metal in suspended solid	
133	Pr-ss	Metal in suspended solid	
134	Nd-ss	Metal in suspended solid	
135	Sm-ss	Metal in suspended solid	
136	Eu-ss	Metal in suspended solid	
137	Gd-ss	Metal in suspended solid	
138	Dy-ss	Metal in suspended solid	
139	Ho-ss	Metal in suspended solid	
140	Er-ss	Metal in suspended solid	
141	Tm-ss	Metal in suspended solid	
142	Yb-ss	Metal in suspended solid	
143	Lu-ss	Metal in suspended solid	
144	Hf-ss	Metal in suspended solid	
145	Ta-ss	Metal in suspended solid	
146	W-ss	Metal in suspended solid	
147	Re-ss	Metal in suspended solid	
148	Pt-ss	Metal in suspended solid	
149	Tl-ss	Metal in suspended solid	
150	^{208}Pb-ss	Metal in suspended solid	
151	Th-ss	Metal in suspended solid	
152	U-plt	Metal in pellet	
153	Ti-plt	Metal in pellet	
154	V-plt	Metal in pellet	
155	^{52}Cr-plt	Metal in pellet	
156	^{53}Cr-plt	Metal in pellet	
157	Mn-plt	Metal in pellet	
158	Fe-plt	Metal in pellet	
159	Co-plt	Metal in pellet	
160	Ni-plt	Metal in pellet	

No.	Variable name	Type	Notes
161	Cu-plt	Metal in pellet	
162	^{66}Zn-plt	Metal in pellet	
163	^{68}Zn-plt	Metal in pellet	
164	Ga-plt	Metal in pellet	
165	Ge-plt	Metal in pellet	
166	As-plt	Metal in pellet	
167	Rb-plt	Metal in pellet	
168	Sr-plt	Metal in pellet	
169	^{95}Mo-plt	Metal in pellet	
170	^{98}Mo-plt	Metal in pellet	
171	Ru-plt	Metal in pellet	
172	Rh-plt	Metal in pellet	
173	Pd-plt	Metal in pellet	
174	^{106}Cd-plt	Metal in pellet	
175	^{111}Cd-plt	Metal in pellet	
176	^{120}Sn-plt	Metal in pellet	
177	Sb-plt	Metal in pellet	
178	Te-plt	Metal in pellet	
179	Cs-plt	Metal in pellet	
180	Ba-plt	Metal in pellet	
181	La-plt	Metal in pellet	
182	Ce-plt	Metal in pellet	
183	Pr-plt	Metal in pellet	
184	Nd-plt	Metal in pellet	
185	Sm-plt	Metal in pellet	
186	Eu-plt	Metal in pellet	
187	Gd-plt	Metal in pellet	
188	Dy-plt	Metal in pellet	
189	Ho-plt	Metal in pellet	
190	Er-plt	Metal in pellet	
191	Tm-plt	Metal in pellet	
192	Yb-plt	Metal in pellet	
193	Lu-plt	Metal in pellet	
194	Hf-plt	Metal in pellet	
195	Ta-plt	Metal in pellet	
196	W-plt	Metal in pellet	
197	Re-plt	Metal in pellet	
198	Pt-plt	Metal in pellet	
199	Tl-plt	Metal in pellet	
200	^{208}Pb-plt	Metal in pellet	
201	Th-plt	Metal in pellet	
202	AODC[1]	Microbial counts	Acridine Orange Direct Count

Notes:

[1] AODC is counted as a microbial measurement rather than a physical-chemical variable, but we still explored its associations with different assembly processes.

Supplementary Table 2 Reference concentrations of stress indicators. Although the reference concentrations are definitely not thresholds of the stress to most microorganisms, we assume that these values could be proportional to the average stress thresholds for microorganisms living in normal conditions. Then, the index calculated as observed concentrations divided by the reference values can be used to assess the relative level of stress. Some other variables (e.g. dissolved oxygen and other heavy metals) can also be stressors, but have no explicit or reported reference level, thus were not included. We assume the stress index based on the following 31 factors can proximately represent the stress level. This is validated by the significant correlation between the maximum stress index and observed number of reference taxa which were common and abundant in uncontaminated areas (Extended Data Fig. 2).

Factor	Abbreviation	Ref. Concentration	Unit	Reference note
Conductivity	Cond.	741	μS/cm	[1]
Hydrogen ion	H^+	$10^{-6.0}$	mol/L	[2]
Hydroxide ion	OH^-	$10^{-6.1}$	mol/L	[2]
Nitrate	NO_3	10	mg-N/L	[3]
Sulfate	SO_4	250	mg/L	[4]
Chloride	Cl	600	mg/L	[4]
Bromine	Br	200	mg/L	[5]
Sodium	Na	3000	mg/L	[6]
Potassium	K	190	mg/L	[6]
Calcium	Ca	130	mg/L	[7]
Magnesium	Mg	170	mg/L	[8]
Aluminum	Al	1.4	mg/L	[9]
Barium	Ba	2	mg/L	[3]
Silver	Ag	0.1	mg/L	[4]
Arsenic	As	0.01	mg/L	[3]
Beryllium	Be	0.004	mg/L	[3]
Bismuth	Bi	0.05	mg/L	[10]
Cadmium	Cd	0.005	mg/L	[3]
Cobalt	Co	0.04	mg/L	[11]
Chromium	Cr	0.12	mg/L	[12]
Caesium	Cs	1.4	mg/L	[13]
Copper	Cu	1.3	mg/L	[3]
Zinc	Zn	5	mg/L	[4]
Iron	Fe	0.3	mg/L	[4]
Manganese	Mn	0.84	mg/L	[14]
Lithium	Li	4	mg/L	[15]
Nickel	Ni	0.15	mg/L	[16]
Lead	Pb	0.02	mg/L	[17]
Selenium	Se	0.05	mg/L	[3]
Strontium	Sr	4.2	mg/L	[18]
Uranium	U	0.03	mg/L	[3]

Notes:

[1] According to "National Secondary Drinking Water Regulations" (US Environmental Protection Agency, 2009, https://www.epa.gov/dwregdev/drinking-water-regulations-and-contaminants#List), Total Dissolved Solids (TDS) should be lower than 500 mg/L. Given the correlation factor from conductivity to TDS ranges from 0.55 to 0.8 (Rusydi AF. Correlation between conductivity and total dissolved solid in various type of water: A review. in IOP Conference Series: Earth and Environmental Science. 2018. doi:10.1088/1755-1315/118/1/012019), we set reference value of conductivity as 741 μS/cm.

[2] According to "Soil Survey Manual" (Soil Survey Division Staff. Chapter 3. Examination and Description of Soils. in Soil survey manual. Soil Conservation Service. U.S. Department of

Agriculture Handbook 18, 1993), the acidic levels higher than moderately acid were defined as pH lower than 6.0, which the alkaline levels higher than moderately alkaline were defined as pH higher than 7.9.

[3] According to "National Primary Drinking Water Regulations" (US Environmental Protection Agency, 2009, https://www.epa.gov/dwregdev/drinking-water-regulations-and-contaminants#List).

[4] According to "National Secondary Drinking Water Regulations".

[5] According to "Tolerance exemptions for active and inert ingredients for use in antimicrobial formulations" (US Environmental Protection Agency. Section 180.940 in Title 40 - Protection of Environment Vol. 23. Code of Federal Regulations, 2006), end-use concentration of all bromide-producing chemicals in the solution should be lower than 200 mg/L.

[6] Human normal serum concentrations of Na and K are 142-145 mmol/L and 3.5-5.0 mmol/L, respectively.

[7] Plasma concentration of symptoms (6.6 mEq/L) for Calcium in Toxnet database (https://toxnet.nlm.nih.gov).

[8] Reported human toxic level (7.1mmol/L) for Magnesium in Toxnet database (https://toxnet.nlm.nih.gov).

[9] According to MAINE State Drinking Water Guidelines (1.43 mg/L), although the value is 0.05~0.2 mg/L in National Secondary Drinking Water Regulations.

[10] Blood no-symptoms level of Bi in Toxnet database (https://toxnet.nlm.nih.gov).

[11] WISCONSIN State Drinking Water Guidelines (Co 40 μg/L).

[12] ARIZONA State Drinking Water Guidelines (Cr 0.12 mg/L), although the value is 0.1 mg/L in National Primary Drinking Water Regulations.

[13] Because animal LD50 level of Cs is the same as Al, we set reference value of Cs the same as Al.

[14] NEW HAMPSHIRE State Drinking Water Guidelines (Mn 0.84 mg/L), although the value is 0.05 mg/L in National Secondary Drinking Water Regulations.

[15] Human toxic effect serum concentration (0.6~1.2 mEq/L) in Toxnet database (https://toxnet.nlm.nih.gov).

[16] ARIZONA State Drinking Water Guidelines (Ni 0.15 mg/L).

[17] ARIZONA State Drinking Water Guidelines (Pb 20 μg/L), although the value is 0.015 mg/L in National Primary Drinking Water Regulations.

[18] FLORIDA State Drinking Water Guidelines (Sr 4.2 mg/L).

Supplementary Table 3 Stress index (SI) of major stressors and the maximum stress index (MSI) of each sample. Each row represents a sample. Stressors with SI always lower than 10 are not included. Stress level A1 to A7 indicate low to extremely high stress. NO_3, nitrate; Cond., conductivity.

Stress Level	MSI	SI of each stressor												
		NO_3	H^+	U	Mn	Ca	OH^-	Al	Cd	Ni	Co	Cond.	Be	Fe
A7	1444.65	1444.65	1.32	2.68	28.29	131.12	0.01	0.04	3.60	1.35	0.44	27.83	9.50	0.00
A7	1347.13	1347.13	33.11	8.65	92.50	100.89	0.00	28.58	61.35	23.16	11.03	25.07	14.23	0.11
A7	906.87	906.87	6.03	299.60	147.71	93.43	0.00	4.14	24.51	6.94	3.35	18.43	10.02	10.66
A7	741.31	0.09	741.31	0.07	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.24	0.00	0.00
A7	585.00	585.00	0.01	0.34	0.05	1.47	1.12	0.04	0.80	0.00	0.00	12.78	9.52	0.04
A7	554.15	269.20	281.84	554.15	38.69	2.10	0.00	77.50	26.46	47.89	12.73	10.61	14.77	0.13
A7	507.76	507.76	19.05	28.39	61.97	56.06	0.00	3.02	64.97	2.32	2.11	12.56	10.14	0.15
A7	459.06	459.06	0.26	0.66	0.16	37.00	0.05	0.03	0.80	0.00	0.08	9.35	9.47	0.00
A7	450.69	450.69	371.54	125.05	152.92	30.54	0.00	81.79	34.53	35.59	30.63	10.75	19.63	0.00
A7	434.07	151.61	204.17	434.07	39.77	0.67	0.00	52.99	33.43	12.13	10.65	4.53	25.16	0.69
A7	375.26	375.26	0.83	1.62	0.12	52.79	0.02	0.00	0.00	0.00	0.47	9.33	0.00	0.00
A7	147.09	147.09	0.15	13.91	9.94	3.23	0.08	0.81	1.31	0.17	0.22	2.32	9.64	15.28
A7	145.54	133.01	83.18	145.54	42.08	1.67	0.00	43.61	26.48	8.34	7.88	3.68	12.68	0.09
A6	140.56	140.56	0.32	0.28	0.03	3.54	0.04	0.00	0.79	0.00	0.00	3.53	9.53	0.09
A6	123.03	0.16	0.00	0.91	0.00	0.00	123.03	0.11	0.81	0.00	0.00	2.20	9.51	0.00
A6	123.03	0.22	0.00	0.16	0.00	0.00	123.03	0.04	0.80	0.00	0.00	3.43	9.50	0.00
A6	97.72	85.05	97.72	28.34	10.48	1.21	0.00	10.84	32.65	1.98	1.60	2.43	10.89	0.00
A6	81.66	81.66	0.33	1.51	0.31	14.27	0.04	0.00	0.00	0.00	0.00	2.30	0.00	0.00
A6	77.62	0.23	0.00	0.72	0.02	0.02	77.62	0.09	0.00	0.00	0.00	0.88	0.00	0.07
A6	73.00	73.00	0.37	0.16	0.20	1.70	0.03	0.03	0.84	0.09	0.00	2.26	9.51	0.00
A6	51.09	0.36	0.26	51.09	0.34	0.97	0.05	0.00	0.00	0.00	0.00	1.14	0.00	0.21
A6	48.41	0.55	0.25	48.41	0.56	0.92	0.05	0.00	0.00	0.00	0.00	0.86	0.00	0.00
A6	47.86	0.14	47.86	0.19	3.15	0.11	0.00	0.23	0.82	0.18	1.72	0.43	9.71	1.02
A6	44.67	0.00	0.00	0.08	0.00	0.00	44.67	0.00	0.00	0.00	0.00	0.62	0.00	0.00
A6	43.70	0.50	0.43	43.70	0.69	0.92	0.03	0.05	0.00	0.00	0.00	1.08	0.00	11.15
A6	42.06	42.06	0.23	1.44	0.13	1.51	0.05	0.03	0.80	0.00	0.00	1.96	9.50	0.00
A5	27.54	0.10	0.00	0.11	0.03	0.21	27.54	0.00	0.40	0.06	0.00	0.52	4.73	0.00
A5	25.70	0.76	0.00	0.31	0.00	0.08	25.70	0.06	0.00	0.00	0.00	0.38	0.00	0.00
A5	24.81	14.10	0.21	24.81	11.18	1.08	0.06	2.46	2.09	1.61	1.39	0.89	0.00	6.44
A5	19.95	0.01	0.00	1.20	0.00	0.00	19.95	0.12	0.00	0.00	0.00	1.14	0.00	0.00
A5	19.50	0.03	0.00	0.07	0.00	0.00	19.50	0.00	0.00	0.00	0.00	1.05	0.00	0.00
A5	19.50	0.00	0.00	0.16	0.00	0.00	19.50	0.30	0.00	0.00	0.00	1.20	0.00	0.00
A5	17.74	0.00	0.40	0.08	17.74	0.39	0.03	0.01	0.00	0.00	0.52	0.61	0.00	0.00
A5	17.10	17.10	5.89	0.63	0.23	0.33	0.00	0.05	0.83	0.11	0.04	0.25	9.54	0.00
A5	16.98	0.04	0.00	1.64	0.06	0.13	16.98	0.06	0.00	0.00	0.00	0.57	0.00	0.00
A5	12.30	1.08	12.30	0.07	0.31	0.24	0.00	0.09	0.00	0.57	0.10	0.81	0.00	0.00
A5	11.85	11.85	10.96	7.83	1.78	0.09	0.00	1.11	3.47	0.31	0.38	0.42	9.75	0.00
A5	9.54	1.34	0.28	1.03	3.15	0.98	0.04	0.05	0.91	0.00	0.05	1.11	9.54	0.07
A5	9.51	0.05	0.20	0.16	0.18	0.37	0.06	0.02	0.79	0.00	0.00	0.47	9.51	0.00
A4	9.49	0.00	0.21	0.19	0.35	0.71	0.06	0.03	0.82	0.00	0.00	0.74	9.49	1.13
A4	9.49	8.41	0.66	0.32	0.22	4.19	0.02	0.02	0.85	0.00	0.00	3.80	9.49	0.00
A4	9.47	0.15	0.09	0.71	0.92	0.85	0.13	0.03	0.82	0.00	0.00	0.78	9.47	1.75
A4	9.33	0.01	0.00	0.27	0.03	0.03	9.33	0.04	0.00	0.00	0.00	0.43	0.00	0.00
A4	7.57	7.57	0.01	1.75	0.04	0.88	0.95	0.01	0.00	0.00	0.00	0.96	0.00	0.00
A4	6.61	0.02	6.61	0.07	0.05	0.00	0.00	0.02	0.00	0.00	0.00	0.05	0.00	0.00
A4	5.62	0.08	5.62	0.21	0.03	0.02	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.00
A4	5.47	5.47	0.05	0.00	0.00	0.65	0.25	0.01	0.00	0.00	0.00	0.49	0.00	0.00
A4	4.96	1.44	0.00	4.96	0.83	0.27	4.68	0.12	0.62	0.00	0.12	0.27	0.00	0.08
A4	4.75	4.75	0.02	0.47	0.00	0.53	0.52	0.01	0.00	0.00	0.00	0.71	0.00	0.00
A4	4.74	0.02	0.30	0.10	0.11	0.69	0.04	0.01	0.40	0.00	0.00	0.78	4.74	2.84

Stress Level	MSI	SI of each stressor												
		NO_3	H^+	U	Mn	Ca	OH^-	Al	Cd	Ni	Co	Cond.	Be	Fe
A4	4.57	0.00	0.23	0.09	0.69	0.98	0.05	0.02	0.00	0.00	0.00	1.08	0.00	4.57
A4	3.98	3.39	3.98	0.07	0.10	0.20	0.00	0.03	0.00	0.47	0.25	0.54	0.00	0.00
A3	3.80	0.00	3.80	0.00	0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.00
A3	3.24	0.00	3.24	0.18	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00
A3	2.88	2.88	0.23	1.36	0.48	0.91	0.05	0.02	0.00	0.00	0.00	1.24	0.00	0.00
A3	2.70	2.70	0.34	0.00	0.00	0.50	0.04	0.01	0.00	0.00	0.00	0.37	0.00	0.00
A3	2.04	0.00	0.01	0.00	0.08	0.21	2.04	0.01	0.00	0.00	0.00	0.33	0.00	0.23
A3	1.95	1.95	0.05	0.95	0.03	0.45	0.25	0.02	0.00	0.00	0.00	0.60	0.00	0.00
A3	1.89	0.00	0.35	0.12	1.34	1.45	0.04	0.01	0.00	0.64	0.00	1.89	0.00	0.21
A3	1.80	0.00	0.37	0.76	1.09	1.76	0.03	0.01	0.00	0.31	0.00	1.80	0.00	0.84
A3	1.47	0.31	0.11	0.76	0.31	0.55	0.11	0.02	0.00	0.00	0.00	1.47	0.00	0.00
A3	1.45	0.02	0.04	0.13	0.48	0.91	0.30	0.11	0.00	0.00	0.00	1.45	0.00	0.29
A3	1.40	0.00	0.15	1.40	0.50	0.60	0.09	0.04	0.62	0.00	0.00	0.63	0.00	0.50
A3	1.35	0.00	0.19	0.14	0.03	0.59	0.07	0.01	0.00	0.00	0.00	1.35	0.00	0.00
A3	1.26	0.14	0.22	0.36	0.60	0.80	0.06	0.02	0.00	0.00	0.00	1.26	0.00	0.00
A2	1.24	0.00	0.21	1.24	0.39	0.95	0.06	0.02	0.00	0.00	0.00	0.86	0.00	0.00
A2	1.22	0.16	0.13	0.15	0.19	0.72	0.10	0.02	0.00	0.00	0.00	1.22	0.00	0.00
A2	1.12	0.02	0.01	0.00	0.01	0.35	1.12	0.01	0.00	0.00	0.00	0.44	0.00	0.00
A2	1.06	1.06	0.26	0.07	0.00	0.45	0.05	0.00	0.00	0.74	0.00	0.51	0.00	0.00
A2	1.06	0.26	0.13	0.24	0.17	0.50	0.09	0.01	0.00	0.16	0.00	1.06	0.00	0.00
A2	0.94	0.00	0.22	0.09	0.60	0.73	0.06	0.00	0.00	0.00	0.00	0.94	0.00	0.00
A2	0.87	0.58	0.87	0.00	0.00	0.28	0.01	0.00	0.00	0.00	0.00	0.63	0.00	0.00
A2	0.84	0.84	0.04	0.14	0.05	0.70	0.30	0.02	0.00	0.00	0.00	0.81	0.00	0.00
A2	0.79	0.50	0.06	0.42	0.10	0.70	0.20	0.02	0.00	0.00	0.00	0.79	0.00	0.00
A2	0.76	0.76	0.06	0.55	0.00	0.55	0.19	0.02	0.00	0.00	0.00	0.48	0.00	0.00
A2	0.75	0.29	0.03	0.08	0.00	0.65	0.42	0.01	0.00	0.00	0.00	0.75	0.00	0.00
A2	0.72	0.33	0.22	0.30	0.22	0.31	0.06	0.02	0.00	0.00	0.00	0.72	0.00	0.00
A2	0.70	0.00	0.02	0.11	0.00	0.50	0.65	0.03	0.00	0.00	0.00	0.70	0.00	0.00
A1	0.69	0.23	0.03	0.24	0.00	0.47	0.38	0.03	0.00	0.00	0.00	0.69	0.00	0.00
A1	0.64	0.04	0.03	0.24	0.30	0.64	0.36	0.00	0.00	0.00	0.00	0.45	0.00	0.00
A1	0.63	0.09	0.63	0.00	0.02	0.10	0.02	0.02	0.00	0.00	0.00	0.09	0.00	0.32
A1	0.63	0.01	0.03	0.11	0.00	0.35	0.36	0.01	0.00	0.00	0.00	0.63	0.00	0.00
A1	0.61	0.03	0.07	0.00	0.01	0.61	0.18	0.01	0.00	0.00	0.00	0.46	0.00	0.00
A1	0.58	0.37	0.09	0.24	0.00	0.46	0.15	0.01	0.00	0.00	0.00	0.58	0.00	0.00
A1	0.55	0.21	0.03	0.16	0.03	0.47	0.39	0.00	0.00	0.00	0.00	0.55	0.00	0.00
A1	0.55	0.06	0.08	0.29	0.06	0.55	0.16	0.00	0.00	0.00	0.00	0.50	0.00	0.07
A1	0.54	0.13	0.54	0.12	0.00	0.18	0.02	0.00	0.00	0.00	0.00	0.16	0.00	0.00
A1	0.53	0.38	0.03	0.31	0.00	0.36	0.39	0.02	0.00	0.00	0.00	0.53	0.00	0.00
A1	0.51	0.00	0.20	0.11	0.00	0.33	0.06	0.02	0.00	0.00	0.00	0.51	0.00	0.00
A1	0.41	0.04	0.05	0.00	0.00	0.40	0.24	0.00	0.00	0.00	0.00	0.41	0.00	0.00
A1	0.36	0.05	0.06	0.00	0.01	0.13	0.19	0.01	0.00	0.00	0.00	0.36	0.00	0.00

Supplementary Table 4 Permutational multivariate analysis of variance (PERMANOVA) for the effect of maximum stress index (MSI) on taxonomic and phylogenetic beta diversity of the bacterial communities.

Factor	**Degree of freedom**	**Sums of Squares**	**Mean of Squares**	**F value**	**R^2**	***P*** (one-sided)
Taxonomic beta diversity (Bray-Curtis)						
MSI	1	0.697	0.697	1.659	0.018	0.004
Residuals	89	37.417	0.420		0.982	
Total	90	38.114			1	
Phylogenetic beta diversity (βMNTD)						
MSI	1	0.016	0.0163	2.930	0.032	0.056
Residuals	89	0.495	0.0056		0.968	
Total	90	0.511			1	

Supplementary Table 5a Taxonomic information of the dominant taxa in the top three phylogenetic bins governed by each major assembly process. Gov. proc., governing process; Ab. Rk., relative abundance rank; HeS, heterogeneous selection; DL, dispersal limitation; DR, drift and other processes.

Gov. Proc.	Ab. Rk.	Bin ID	Dominant taxon ID	Phylum	Class	Order	Family	Genus	Species
HeS	1	Bin37	136638	WPS-2	Unclassified	Unclassified	Unclassified	Unclassified	Unclassified
	2	Bin101	4418129	Unclassified	Unclassified	Unclassified	Unclassified	Unclassified	Unclassified
	3	Bin256	226074	RCP2-54	Unclassified	Unclassified	Unclassified	Unclassified	Unclassified
DL	1	Bin154	738779	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Unclassified	Unclassified
	2	Bin23	NR8426	Bacteroidota	Kryptonia	Kryptoniales	BSV26	BSV26	Uncultured bacterium
	3	Bin137	638460	Proteobacteria	Gammaproteobacteria	Burkholderiales	Gallionellaceae	Unclassified	Unclassified
DR	1	Bin130	1106617	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified	Unclassified
	2	Bin223	841170	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Brevundimonas	Unclassified
	3	Bin129	1108726	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified	Unclassified

Supplementary Table 5b NCBI top hits of the dominant taxa in the top three phylogenetic bins governed by each major assembly process. Ident., identity; cul., include culturable strain(s) or not.

Gov. Proc.	Bin ID	Dominant taxon ID	NCBI Accession No.	Ident.	Cover	Source habitats	Cul.?
HeS	Bin37	136638	DQ125709.1; DQ125594.1; DQ125902.1; KC786515.1	100%	100%	Uranium contaminated soil (FRC Area 2, three clones); Wastewater-impacted riparian buffer zone	No
			DQ125859.1, DQ125774.1, DQ125647.1; EF175358.1	99.60%	100%	Uranium contaminated soil (FRC Area 2, three clones); nitrate and uranium contaminated sediment	No
	Bin101	4418129	AB746521.1	100%	100%	Deep Granitic Groundwater	No
			KC575050.1; KC574889.1; AB746490.1; AB746489.1	99.60%	100%	An ultrabasic, ultrareducing, and low salinity serpentinizing spring; Deep groundwater.	No
			KX163991.1; KX163990.1; KC575053.1; KC575052.1; AB746494.1; AB179681.1	99.21%	100%	A deep basaltic aquifer; An ultrabasic, ultrareducing, and low salinity serpentinizing spring; Deep groundwater (pass through 0.2-micrometer-pore-size filter)	No
	Bin256	226074	KP907134.1; JQ366238.2	99.21%	100%	Post-volcanic pyroclastic surface; Soil exposed to 10 years of elevated atmospheric carbon dioxide	No
DL	Bin154	738779	MN156637.1; MF081585.1	99.60%	100%	Anaerobic digester	Yes
			MH445104.1; MG016388.1; KU685498.1; KU685489.1; KX163889.1; LC122006.1; LC094772.1; KJ831771.1; KJ807868.1; KJ807868.1; KJ877470.1; KF810120.1; KF810119.1; KF810116.1; KF697602.1; KC110516.1, etc.	99.21%	100%	Soil; Paddy soil; Rhizospheric soil; Rhizosphere of constructed wetland; Deep aquifer under anthropogenic CO2 injection; Deep aquifers; Anammox bioreactor; Aerobic activated sludge; Aerobic and anaerobic bioreactors; Wastewater; Groundwater	Yes
	Bin23	NR8426	MH112962.1	99.21%	100%	Eutrophic lakes with oxygen-deprived bottom waters	No
	Bin137	638460	MK521793.1; MH524929.1; KX957309.1; KU221802.1; KP688856.1; KU587047.1; JQ217785.1; JQ217653.1 etc.	96.50%	100%	Acidic Pit Lake; Forest soil; Bay sediment; Acidic mine stalactite and drainage; Goethite precipitation from pH neutral water; Soil	No

Gov. Proc.	Bin ID	Dominant taxon ID	NCBI Accession No.	Ident.	Cover	Source habitats	Cul.?
DR	Bin130	1106617	KY890604.1; MH524670.1; MG715791.1; KU151873.1; MF555781.1; MF363864.1; KU482628.1; KU480089.1; KJ633601.1; LN532109.1; KF066376.1; KF638288.1; KC786310.1	100%	100%	Soil from restored wetlands; Forest Soil; Groundwater; Hot springs; Waste deposit soil; Rapid sand filter material in drinking water treatment; Human skin and nare; Maize rhizosphere; Riparian buffer zone soil	Yes
	Bin223	841170	JQ791565.1; JQ669873.1; FN821834.1	100%	100%	Biofilm in dinking water; compost based column remediating Cr(VI)-contaminated groundwater; Bank-filtered raw water	Yes
			KT908721.1; HQ904741.1; HQ904741.1	99.60%	100%	River biofilm; Particle-attached bacterial sample from lake	
			LC466873.1; MH312570.1; MH228377.1; MG966306.1 etc.	99.21	100%	Cucumber pickles; River sediment; Feces; River and lake water; Groundwater; Seawater and sediment; Hot springs; Soil.	
	Bin129	1108726	AB835627.1; AB672320.1; LC435926.1; LC435925.1; MK726429.1; MH524669.1; KY892321.1; KU461282.1; KM138797.1; KC574957.1; KC355350.1; HF543718.1; JQ480461.1 etc.	100%	100%	Forest soil; Paddy Soil; Ectomycorrhizal root tip; Plant root; Soil from restored wetlands; Hot springs; Lake; Serpetinizing springs; Fresh water; Glacier forefield, etc.	Yes

Supplementary Table 5c Detected 16S rRNA sequences of the dominant taxa in the top phylogenetic bins governed by each major process.

BinID	Dominant taxon ID	Sequence
Bin37	136638	GACGTAGGGGGCGAGCGTTGTTCGGAATCATTGGGCGTAAAGCGCGCGTAGGCGGACAGCAAGTCTGTGAAGAAAGACCCCGGCTTAACTGGGGGACCGGCATAGATACTGTTGTTCTTGAGATGGTCAGAGGGTGATGGAATTCCCGGTGTAGCGGTGAAATGCGTAGATATCGGGAGGAACACCAGTGGCGAAGGCGATCACCTGGGGCTAATCTGACGCTGAGGCGCGAAAGCTAGGGGAGCAAACGGG
Bin101	4418129	TACGTGGGTGGCGAGCGTTATCCGGATTTACTGGGCGTAAAGGGCCTGCAGGTGGTTCCTAAAGTCCCCGGTAAAATCTTAAGGCCTAACCTTAAGAAGACTGGGGATACTCAGGAGCTAGAGGAAAGGAGAGGGAAGTGGAATTCCTGGTGGAGCGGTGAAATGCGTAGATATCAGGAGGAACACCCAAGGCGAAGGCAGCTTCCTGGCCTTTTCCTGACACTCAGAGGCGAAAGCTGGGGGAGCAAACGGG
Bin256	226074	GACGGAGGGTGCAAGCGTTGTTCGGATTGACTGGGCGTAAAGGGCGTGTAGGCGGTTGGTCAAGTCTGATGTGAAAGCCCGGGGCTCAGCTCCGGAAGTGCGTCGGAAACTAGCCAGCTGGAGCGCGATAGAGGAGAGTGGAATTCCTGGTGTAGCGGTGAAATGCGTAGATATCAGGAGGAACACCGGCGGCGAAGGCGGCTCTCTGGATCGTTGCTGACGCTGAGACGCGAAAGCGTGGGGAGCAAACAGG
Bin154	738779	TACGTAGGGTGCGAGCGTTAATCGGAATTACTGGGCGTAAAGCGTGCGCAGGCGGTTTTGTAAGACAGGTGTGAAATCCCCGGGCTTAACCTGGGAACTGCGCTTGTGACTGCAAGACTGGAGTGCGGCAGAGGGGGGTGGAATTCCACGTGTAGCAGTGAAATGCGTAGAGATGTGGAGGAACACCGATGGCGAAGGCAGCCCCCTGGGTCGACACTGACGCTCAGGCACGAAAGCGTGGGGAGCAAACAGG
Bin23	NR8426	TACGTAGGATCCGAGCGTTGTCCGGATTTACTGGGTGTAAAGGGAGCGCAGGCGGACTTTTAAGTCGGTGGTGAAATCTCGAAGCTTAACTTCGAAACTGCTTCCGAAACTATTAGTCTTGAATCTAGAAGAGGGCGATGGAATTCATGGTGTAGCAGTAAAATGCGTAGATATCATGAAGAACACCAGTCGCGAAGGCGGTCGCCTGGTCTAGTATTAACGCTCATGCTCGAAAGTGTGGGGAGCAAACAGG

BinID	Dominant taxon ID	Sequence
Bin137	638460	TACGTAGGGTGCGAGCGTTAATCGGAATTACTGGGCGTAAAGCGTGCGCAGGCGGTTTTGTAAGAAGCGCGAAATCCCCGGGCTTAACTTGGGAATGCGTTTGGACTGCAAGACTAGAGTCGGCAGAGGGGGGTAGAATTCCACGTGTAGCAGTGAAATGCGTAGATATGTGGAGGAATACCGATGGCGAAGGCAGCCCCCTGGGTGAACTGACGCTTATGCACGAAAGCGTGGGGAGCAAACAGG
Bin130	1106617	TACGTAGGGTGCAAGCGTTAATCGGAATTACTGGGCGTAAAGCGTGCGCAGGCGGTTATGTAAGACAGGTGTGAAATCCCCGGGCTTAACCTGGGAACTGCATTTGTGACTGCATAGCTAGAGTACGGTAGAGGGGGATGGAATTCCGCGTGTAGCAGTGAAATGCGTAGATATGCGGAGGAACACCGATGGCGAAGGCAATCCCCTGGACCTGTACTGACGCTCATGCACGAAAGCGTGGGGAGCAAACAGG
Bin223	841170	TACGAAGGGGGCTAGCGTTGCTCGGAATTACTGGGCGTAAAGGGAGCGTAGGCGGACATTTAAGTCAGAGGTGAAATCCCGGGGCTCAACCTCGGAACTGCCTTTGATACTGGATGTCTTGAGTGTGAGAGAGGTATGTGGAACTCCGAGTGTAGAGGTGAAATTCGTAGATATTCGGAAGAACACCAGTGGCGAAGGCGACATACTGGCTCATTACTGACGCTGAGGCTCGAAAGCGTGGGGAGCAAACAGG
Bin129	1108726	TACGTAGGGTGCAAGCGTTAATCGGAATTACTGGGCGTAAAGCGTGCGCAGGCGGTTCTATAAGACAGATGTGAAATCCCCGGGCTCAACCTGGGAACTGCATTTGTGACTGTAGAGCTGGAGTGCGGCAGAGGGGGATGGAATTCCGCGTGTAGCAGTGAAATGCGTAGATATGCGGAGGAACACCGATGGCGAAGGCAATCCCCTGGGCCTGCACTGACGCTCATGCACGAAAGCGTGGGGAGCAAACAGG

Supplementary Table 6 Coefficient of determination between each environmental variable and the relative importance of each assembly process based on cross-validated Mantel test. -sup, in supernatant; -ss, in suspended solid; -plt, in pellet. The cross-validated coefficients of determination (R^2_{CV}) are outside the parentheses, and *P* values (one-sided) are in the parentheses.

Environmental variable	**Heterogeneous Selection**	**Homogeneous Selection**	**Dispersal Limitation**	**Homogenizing Dispersal**	**'Drift'**
Geographic distance	-0.0067(0.180)	-0.0077(0.051)	-0.0074(0.364)	-0.0081(0.110)	-0.0116(0.422)
Elevation	0.0086(0.005)	-0.0025(0.001)	-0.0202(0.055)	-0.0054(0.035)	-0.0224(0.116)
Depth (T)	-0.0049(0.030)	0.0056(0.001)	-0.0135(0.243)	-0.0112(0.305)	-0.0113(0.130)
Depth (B)	0.0033(0.008)	0.0126(0.001)	-0.0088(0.080)	-0.0082(0.103)	-0.0095(0.067)
Screen	-0.0078(0.077)	0.0052(0.001)	-0.0117(0.270)	-0.0140(0.277)	-0.0133(0.186)
Conductivity	0.0152(0.003)	-0.0136(0.111)	-0.0178(0.259)	-0.0196(0.137)	-0.0136(0.069)
Temperature	-0.0098(0.144)	-0.0095(0.094)	-0.0054(0.015)	-0.0065(0.140)	-0.0126(0.442)
pH	0.1258(0.001)	0.0064(0.001)	-0.0113(0.039)	0.0126(0.002)	-0.0194(0.421)
Redox	-0.0209(0.200)	-0.0234(0.466)	-0.0202(0.067)	-0.0258(0.480)	-0.0210(0.331)
DO	-0.0189(0.406)	-0.0148(0.203)	-0.0171(0.340)	-0.0151(0.127)	-0.0163(0.118)
DIC	0.0360(0.001)	-0.0094(0.029)	-0.0112(0.072)	-0.0056(0.024)	-0.0139(0.304)
DOC	0.0278(0.001)	-0.0042(0.002)	-0.0137(0.111)	-0.0001(0.009)	-0.0197(0.273)
O_2	-0.0225(0.365)	-0.0189(0.193)	-0.0177(0.414)	-0.0228(0.423)	-0.0219(0.464)
CH_4	-0.0051(0.031)	-0.0176(0.114)	-0.0189(0.404)	-0.0184(0.280)	-0.0026(0.038)
CO_2	0.0451(0.001)	0.0086(0.002)	-0.0075(0.025)	0.0108(0.001)	-0.0138(0.178)
N_2	-0.0223(0.289)	-0.0212(0.400)	-0.0199(0.191)	-0.0286(0.448)	-0.0232(0.334)
N_2O	0.0455(0.001)	-0.0111(0.129)	-0.0177(0.211)	0.0030(0.003)	-0.0200(0.431)
Sulfide	-0.0035(0.032)	-0.0072(0.307)	-0.0058(0.111)	-0.0062(0.202)	-0.0074(0.285)
Cl	-0.0120(0.496)	-0.0096(0.207)	-0.0098(0.106)	-0.0040(0.096)	-0.0072(0.092)
Br	0.0060(0.003)	-0.0012(0.004)	-0.0060(0.281)	0.0012(0.003)	0.0030(0.003)
NO_3	0.0303(0.001)	-0.0041(0.014)	-0.0102(0.244)	0.0004(0.018)	-0.0127(0.314)
PO_4	-0.0100(0.030)	-0.0212(0.227)	-0.0239(0.213)	-0.0231(0.356)	-0.0197(0.184)
SO_4	0.0317(0.003)	-0.0128(0.009)	-0.0165(0.034)	0.0111(0.006)	-0.0183(0.132)
NO_2	-0.0062(0.101)	-0.0100(0.137)	-0.0103(0.174)	-0.0078(0.076)	-0.0107(0.192)
Fe(II)	-0.0046(0.081)	-0.0053(0.039)	-0.0072(0.372)	-0.0065(0.245)	-0.0077(0.270)
K	0.0360(0.001)	-0.0162(0.108)	-0.0133(0.072)	-0.0044(0.025)	-0.0189(0.296)
Na	0.0121(0.002)	-0.0020(0.013)	-0.0039(0.150)	0.0016(0.003)	-0.0047(0.395)
Ca	0.0762(0.001)	-0.0018(0.002)	-0.0131(0.093)	0.0156(0.004)	-0.0246(0.396)
Mg	-0.0060(0.030)	-0.0198(0.401)	-0.0209(0.420)	-0.0168(0.067)	-0.0293(0.299)
Al	0.0615(0.001)	-0.0161(0.253)	-0.0038(0.001)	-0.0054(0.025)	-0.0192(0.146)
Ba	-0.0021(0.020)	-0.0151(0.170)	-0.0198(0.324)	-0.0200(0.168)	-0.0172(0.240)
Ag	-0.0234(0.405)	-0.0224(0.286)	-0.0197(0.346)	-0.0182(0.205)	-0.0119(0.092)
As	-0.0256(0.380)	-0.0215(0.340)	-0.0217(0.442)	-0.0197(0.197)	-0.0038(0.031)
Be	0.0355(0.001)	-0.0094(0.102)	-0.0051(0.022)	0.0053(0.001)	-0.0104(0.326)
Bi	-0.0314(0.447)	-0.0241(0.230)	-0.0234(0.374)	-0.0228(0.357)	-0.0323(0.292)
Cd	0.0734(0.001)	-0.0122(0.097)	-0.0116(0.020)	0.0140(0.002)	-0.0199(0.466)
Co	0.1221(0.001)	-0.0089(0.010)	-0.0104(0.033)	0.0193(0.001)	-0.0188(0.402)
Cr	-0.0023(0.061)	-0.0044(0.163)	-0.0052(0.483)	-0.0036(0.226)	-0.0049(0.337)
Cs	0.0142(0.001)	-0.0091(0.156)	-0.0074(0.204)	-0.0029(0.019)	-0.0105(0.243)
Cu	-0.0072(0.271)	-0.0069(0.279)	-0.0054(0.120)	-0.0053(0.105)	0.0070(0.007)
Zn	0.0472(0.002)	-0.0143(0.166)	-0.0082(0.005)	-0.0039(0.032)	-0.0208(0.479)
Fe	-0.0105(0.083)	-0.0131(0.457)	-0.0109(0.095)	-0.0174(0.462)	-0.0028(0.030)
Ga	0.0012(0.024)	-0.0029(0.029)	-0.0061(0.406)	-0.0081(0.355)	-0.0031(0.084)
Mn	0.0527(0.001)	0.0029(0.001)	-0.0091(0.428)	0.0070(0.002)	-0.0101(0.326)
Li	0.0332(0.001)	-0.0043(0.030)	-0.0034(0.012)	0.0016(0.007)	-0.0092(0.452)
Ni	0.0581(0.001)	-0.0156(0.101)	-0.0135(0.018)	0.0064(0.006)	-0.0191(0.402)
Pb	0.0315(0.001)	-0.0066(0.010)	-0.0048(0.026)	-0.0009(0.018)	-0.0090(0.421)
Se	-0.0203(0.067)	-0.0210(0.414)	-0.0176(0.041)	-0.0434(0.327)	-0.0289(0.135)

Environmental variable	Heterogeneous Selection	Homogeneous Selection	Dispersal Limitation	Homogenizing Dispersal	'Drift'
Sr	-0.0184(0.335)	-0.0182(0.457)	-0.0174(0.136)	-0.0190(0.096)	0.0234(0.001)
U	0.0184(0.003)	-0.0150(0.117)	-0.0120(0.030)	-0.0158(0.240)	-0.0060(0.037)
U-sup	0.0375(0.001)	-0.0151(0.191)	-0.0147(0.082)	0.0046(0.006)	-0.0149(0.427)
Ti-sup	0.0599(0.001)	-0.0113(0.015)	-0.0167(0.422)	0.0095(0.002)	-0.0188(0.468)
V-sup	-0.0085(0.037)	-0.0213(0.277)	-0.0222(0.162)	-0.0192(0.299)	-0.0163(0.132)
^{52}Cr-sup	-0.0147(0.463)	-0.0131(0.220)	-0.0119(0.136)	-0.0141(0.357)	-0.0124(0.160)
^{53}Cr-sup	-0.0167(0.220)	-0.0160(0.403)	-0.0176(0.302)	-0.0177(0.472)	-0.0156(0.165)
Mn-sup	0.0626(0.001)	0.0017(0.002)	-0.0090(0.377)	0.0157(0.001)	-0.0092(0.166)
Fe-sup	0.0459(0.001)	-0.0075(0.002)	-0.0159(0.478)	0.0053(0.007)	-0.0176(0.250)
Co-sup	0.0507(0.001)	-0.0073(0.015)	-0.0134(0.324)	0.0108(0.001)	-0.0107(0.127)
Ni-sup	0.0319(0.001)	-0.0142(0.101)	-0.0155(0.285)	0.0141(0.005)	-0.0163(0.159)
Cu-sup	0.0115(0.001)	-0.0064(0.115)	-0.0063(0.396)	0.0050(0.007)	-0.0018(0.063)
^{66}Zn-sup	-0.0218(0.415)	-0.0183(0.336)	-0.0150(0.274)	-0.0165(0.339)	-0.0246(0.471)
^{68}Zn-sup	0.0045(0.015)	-0.0083(0.021)	-0.0080(0.022)	-0.0070(0.039)	-0.0186(0.500)
Ga-sup	-0.0201(0.158)	-0.0157(0.180)	-0.0205(0.294)	-0.0202(0.235)	-0.0228(0.459)
Ge-sup	0.0095(0.004)	-0.0081(0.007)	-0.0051(0.002)	-0.0299(0.441)	-0.0176(0.216)
As-sup	0.0053(0.001)	0.0006(0.001)	-0.0025(0.461)	-0.0005(0.018)	0.0001(0.010)
Rb-sup	-0.0158(0.184)	-0.0114(0.373)	-0.0137(0.411)	-0.0162(0.261)	-0.0140(0.215)
Sr-sup	-0.0101(0.125)	-0.0163(0.408)	-0.0155(0.190)	-0.0191(0.420)	-0.0109(0.061)
^{95}Mo-sup	0.0709(0.001)	-0.0084(0.012)	-0.0027(0.001)	-0.0040(0.015)	-0.0179(0.369)
^{98}Mo-sup	0.0740(0.001)	-0.0112(0.025)	-0.0024(0.001)	-0.0034(0.017)	-0.0221(0.419)
Ru-sup	-0.0087(0.306)	-0.0072(0.348)	-0.0076(0.358)	-0.0076(0.270)	-0.0076(0.270)
Rh-sup	-0.0077(0.375)	-0.0061(0.120)	-0.0072(0.136)	-0.0093(0.261)	-0.0084(0.286)
Pd-sup	0.0004(0.009)	-0.0014(0.134)	-0.0017(0.316)	-0.0013(0.275)	-0.0013(0.152)
^{106}Cd-sup	-0.0021(0.031)	-0.0085(0.149)	-0.0085(0.395)	-0.0081(0.161)	-0.0096(0.446)
^{111}Cd-sup	0.0533(0.002)	-0.0144(0.260)	-0.0150(0.019)	0.0194(0.002)	-0.0179(0.120)
^{120}Sn-sup	-0.0001(0.004)	-0.0017(0.191)	-0.0008(0.132)	-0.0008(0.027)	-0.0006(0.079)
Sb-sup	-0.0158(0.282)	-0.0121(0.303)	-0.0147(0.463)	-0.0160(0.421)	-0.0147(0.502)
Te-sup	0.0092(0.001)	-0.0007(0.002)	-0.0028(0.100)	-0.0005(0.008)	-0.0027(0.157)
Cs-sup	-0.0145(0.185)	-0.0126(0.140)	-0.0148(0.141)	-0.0150(0.286)	-0.0161(0.108)
Ba-sup	-0.0102(0.043)	-0.0167(0.127)	-0.0183(0.341)	-0.0171(0.180)	-0.0230(0.490)
La-sup	0.0786(0.001)	-0.0129(0.100)	-0.0121(0.013)	0.0179(0.002)	-0.0188(0.214)
Ce-sup	0.0455(0.001)	-0.0141(0.100)	-0.0109(0.023)	0.0141(0.005)	-0.0139(0.184)
Pr-sup	0.0159(0.002)	-0.0137(0.412)	-0.0107(0.017)	0.0034(0.022)	-0.0112(0.162)
Nd-sup	0.0374(0.001)	-0.0039(0.005)	-0.0034(0.006)	0.0002(0.017)	-0.0116(0.258)
Sm-sup	0.0479(0.001)	-0.0057(0.010)	-0.0033(0.003)	-0.0014(0.011)	-0.0113(0.305)
Eu-sup	0.0744(0.001)	-0.0125(0.046)	-0.0055(0.001)	0.0023(0.008)	-0.0196(0.529)
Gd-sup	0.0790(0.001)	-0.0171(0.095)	-0.0096(0.005)	0.0188(0.001)	-0.0197(0.133)
Dy-sup	0.0261(0.002)	-0.0144(0.326)	-0.0100(0.048)	0.0091(0.001)	-0.0143(0.123)
Ho-sup	0.0437(0.001)	-0.0127(0.234)	-0.0099(0.018)	0.0150(0.004)	-0.0154(0.187)
Er-sup	0.0419(0.001)	-0.0057(0.020)	-0.0041(0.007)	0.0044(0.005)	-0.0100(0.300)
Tm-sup	0.0256(0.001)	-0.0080(0.055)	-0.0053(0.022)	0.0046(0.003)	-0.0036(0.040)
Yb-sup	0.0410(0.001)	-0.0059(0.035)	-0.0030(0.005)	0.0020(0.009)	-0.0109(0.462)
Lu-sup	-0.0069(0.116)	-0.0103(0.426)	-0.0081(0.023)	-0.0109(0.509)	-0.0087(0.212)
Hf-sup	0.0095(0.007)	-0.0171(0.511)	-0.0138(0.095)	-0.0101(0.046)	-0.0192(0.249)
Ta-sup	-0.0120(0.155)	-0.0111(0.343)	-0.0089(0.022)	-0.0130(0.526)	-0.0081(0.114)
W-sup	-0.0022(0.121)	-0.0021(0.150)	-0.0027(0.415)	-0.0031(0.216)	-0.0015(0.089)
Re-sup	-0.0086(0.091)	-0.0130(0.293)	-0.0124(0.064)	-0.0166(0.392)	-0.0077(0.055)
Pt-sup	-0.0114(0.078)	-0.0128(0.241)	-0.0162(0.361)	-0.0081(0.055)	-0.0205(0.429)
Tl-sup	0.0122(0.008)	-0.0102(0.064)	-0.0100(0.180)	-0.0083(0.081)	-0.0142(0.432)
^{208}Pb-sup	-0.0105(0.289)	-0.0080(0.052)	-0.0097(0.062)	-0.0135(0.316)	-0.0155(0.222)
Th-sup	-0.0059(0.059)	-0.0142(0.287)	-0.0166(0.375)	-0.0121(0.118)	-0.0165(0.429)
U-ss	0.0304(0.001)	-0.0122(0.337)	-0.0143(0.128)	0.0047(0.006)	-0.0167(0.462)
Ti-ss	0.0261(0.002)	-0.0115(0.047)	-0.0164(0.459)	-0.0010(0.012)	-0.0169(0.469)
V-ss	-0.0128(0.459)	-0.0125(0.248)	-0.0127(0.484)	-0.0131(0.352)	-0.0121(0.385)
^{52}Cr-ss	-0.0156(0.305)	-0.0111(0.378)	-0.0105(0.394)	-0.0128(0.272)	-0.0154(0.392)

Environmental variable	**Heterogeneous Selection**	**Homogeneous Selection**	**Dispersal Limitation**	**Homogenizing Dispersal**	**‘Drift’**
^{53}Cr-ss	-0.0098(0.102)	-0.0138(0.411)	-0.0130(0.328)	-0.0139(0.267)	-0.0138(0.310)
Mn-ss	0.0600(0.001)	0.0042(0.001)	-0.0131(0.438)	0.0167(0.001)	-0.0131(0.233)
Fe-ss	-0.0078(0.091)	-0.0097(0.203)	-0.0064(0.060)	-0.0057(0.070)	-0.0104(0.344)
Co-ss	0.0897(0.001)	-0.0099(0.017)	-0.0154(0.050)	0.0251(0.001)	-0.0178(0.249)
Ni-ss	0.0472(0.001)	-0.0164(0.255)	-0.0132(0.044)	0.0288(0.002)	-0.0128(0.065)
Cu-ss	-0.0074(0.060)	-0.0145(0.424)	-0.0171(0.072)	-0.0140(0.136)	-0.0165(0.339)
^{66}Zn-ss	-0.0226(0.267)	-0.0176(0.196)	-0.0165(0.383)	-0.0168(0.428)	-0.0221(0.447)
^{68}Zn-ss	0.0032(0.027)	-0.0054(0.010)	-0.0113(0.023)	-0.0129(0.089)	-0.0231(0.403)
Ga-ss	-0.0100(0.075)	-0.0156(0.090)	-0.0179(0.311)	-0.0219(0.366)	-0.0164(0.180)
Ge-ss	-0.0023(0.040)	-0.0142(0.074)	-0.0105(0.211)	-0.0117(0.155)	-0.0149(0.196)
As-ss	-0.0248(0.461)	-0.0219(0.193)	-0.0189(0.116)	-0.0173(0.211)	-0.0080(0.035)
Rb-ss	-0.0113(0.130)	-0.0132(0.453)	-0.0130(0.378)	-0.0155(0.234)	-0.0154(0.269)
Sr-ss	-0.0079(0.062)	-0.0167(0.418)	-0.0166(0.161)	-0.0215(0.304)	-0.0088(0.087)
^{95}Mo-ss	0.0372(0.001)	-0.0081(0.010)	-0.0065(0.004)	-0.0173(0.127)	-0.0249(0.290)
^{98}Mo-ss	0.0313(0.001)	-0.0074(0.015)	-0.0067(0.006)	-0.0218(0.230)	-0.0230(0.129)
Ru-ss	-0.0071(0.177)	-0.0080(0.184)	-0.0054(0.028)	-0.0068(0.222)	-0.0084(0.238)
Rh-ss	-0.0109(0.254)	-0.0088(0.233)	-0.0062(0.018)	-0.0101(0.224)	-0.0123(0.318)
Pd-ss	0.0072(0.001)	-0.0038(0.010)	-0.0055(0.318)	-0.0044(0.102)	-0.0036(0.077)
^{106}Cd-ss	0.0269(0.002)	-0.0181(0.185)	-0.0171(0.044)	0.0021(0.010)	-0.0303(0.351)
^{111}Cd-ss	0.0300(0.001)	-0.0141(0.477)	-0.0122(0.023)	0.0099(0.003)	-0.0208(0.214)
^{120}Sn-ss	-0.0082(0.207)	-0.0040(0.015)	-0.0080(0.139)	-0.0088(0.252)	-0.0066(0.176)
Sb-ss	-0.0145(0.259)	-0.0106(0.161)	-0.0128(0.399)	-0.0145(0.360)	-0.0138(0.421)
Te-ss	-0.0029(0.098)	-0.0040(0.398)	-0.0040(0.424)	-0.0046(0.136)	-0.0039(0.498)
Cs-ss	-0.0114(0.156)	-0.0130(0.213)	-0.0160(0.457)	-0.0192(0.405)	-0.0159(0.283)
Ba-ss	-0.0101(0.045)	-0.0184(0.175)	-0.0202(0.307)	-0.0150(0.135)	-0.0232(0.485)
La-ss	0.0440(0.001)	-0.0141(0.140)	-0.0150(0.019)	0.0069(0.004)	-0.0218(0.190)
Ce-ss	0.0361(0.002)	-0.0144(0.108)	-0.0139(0.040)	0.0076(0.004)	-0.0175(0.191)
Pr-ss	0.0200(0.001)	-0.0139(0.192)	-0.0134(0.026)	-0.0011(0.009)	-0.0191(0.125)
Nd-ss	0.0391(0.002)	-0.0147(0.178)	-0.0110(0.011)	0.0037(0.009)	-0.0189(0.232)
Sm-ss	0.0422(0.001)	-0.0156(0.120)	-0.0084(0.019)	0.0060(0.005)	-0.0187(0.263)
Eu-ss	0.0748(0.001)	-0.0139(0.101)	-0.0080(0.010)	0.0022(0.006)	-0.0204(0.441)
Gd-ss	0.0378(0.001)	-0.0157(0.179)	-0.0127(0.021)	0.0052(0.005)	-0.0195(0.223)
Dy-ss	0.0451(0.001)	-0.0041(0.015)	-0.0059(0.019)	0.0061(0.003)	-0.0118(0.205)
Ho-ss	0.0091(0.010)	-0.0193(0.371)	-0.0164(0.087)	-0.0045(0.022)	-0.0189(0.176)
Er-ss	0.0272(0.004)	-0.0181(0.226)	-0.0144(0.029)	0.0095(0.006)	-0.0194(0.202)
Tm-ss	0.0123(0.003)	-0.0131(0.432)	-0.0107(0.029)	0.0043(0.008)	-0.0117(0.108)
Yb-ss	0.0380(0.001)	-0.0145(0.293)	-0.0071(0.018)	0.0047(0.002)	-0.0178(0.186)
Lu-ss	0.0022(0.009)	-0.0086(0.064)	-0.0104(0.474)	-0.0086(0.198)	-0.0102(0.191)
Hf-ss	-0.0025(0.039)	-0.0125(0.106)	-0.0112(0.026)	-0.0188(0.307)	-0.0058(0.024)
Ta-ss	0.0209(0.001)	-0.0062(0.178)	-0.0048(0.089)	0.0017(0.004)	-0.0082(0.412)
W-ss	-0.0002(0.013)	-0.0043(0.187)	-0.0044(0.211)	-0.0025(0.093)	-0.0055(0.408)
Re-ss	-0.0041(0.035)	-0.0149(0.176)	-0.0121(0.045)	-0.0136(0.156)	-0.0110(0.208)
Pt-ss	-0.0136(0.205)	-0.0126(0.338)	-0.0093(0.039)	-0.0146(0.459)	-0.0108(0.170)
Tl-ss	-0.0217(0.480)	-0.0155(0.206)	-0.0060(0.006)	-0.0178(0.321)	-0.0130(0.481)
^{208}Pb-ss	-0.0208(0.294)	-0.0177(0.500)	-0.0230(0.221)	-0.0140(0.114)	-0.0146(0.081)
Th-ss	-0.0071(0.058)	-0.0149(0.184)	-0.0168(0.270)	-0.0139(0.176)	-0.0142(0.140)
U-plt	0.0013(0.021)	-0.0156(0.307)	-0.0170(0.270)	-0.0102(0.042)	-0.0230(0.224)
Ti-plt	-0.0094(0.363)	-0.0075(0.464)	-0.0053(0.051)	-0.0060(0.171)	-0.0081(0.223)
V-plt	-0.0146(0.152)	-0.0146(0.027)	-0.0151(0.101)	-0.0192(0.163)	-0.0187(0.094)
^{52}Cr-plt	-0.0177(0.346)	-0.0170(0.237)	-0.0117(0.095)	-0.0197(0.430)	-0.0136(0.150)
^{53}Cr-plt	-0.0211(0.488)	-0.0126(0.465)	-0.0114(0.038)	-0.0172(0.411)	-0.0137(0.218)
Mn-plt	-0.0013(0.026)	-0.0092(0.327)	-0.0091(0.475)	-0.0057(0.071)	-0.0112(0.500)
Fe-plt	-0.0029(0.045)	-0.0072(0.253)	-0.0049(0.073)	-0.0020(0.022)	-0.0083(0.281)
Co-plt	-0.0086(0.063)	-0.0121(0.310)	-0.0119(0.085)	-0.0134(0.265)	-0.0167(0.436)
Ni-plt	-0.0083(0.235)	-0.0082(0.315)	-0.0089(0.259)	-0.0081(0.277)	-0.0112(0.473)
Cu-plt	-0.0154(0.154)	-0.0142(0.062)	-0.0202(0.262)	-0.0195(0.246)	-0.0212(0.317)

Environmental variable	**Heterogeneous Selection**	**Homogeneous Selection**	**Dispersal Limitation**	**Homogenizing Dispersal**	**‘Drift’**
^{66}Zn-plt	-0.0086(0.246)	-0.0081(0.258)	-0.0080(0.447)	-0.0081(0.430)	-0.0090(0.473)
^{68}Zn-plt	-0.0044(0.029)	-0.0113(0.379)	-0.0099(0.255)	-0.0069(0.059)	-0.0087(0.190)
Ga-plt	-0.0128(0.080)	-0.0134(0.409)	-0.0146(0.171)	-0.0133(0.115)	-0.0156(0.149)
Ge-plt	-0.0095(0.370)	-0.0070(0.208)	-0.0047(0.037)	-0.0100(0.380)	-0.0088(0.158)
As-plt	-0.0056(0.156)	-0.0041(0.067)	-0.0036(0.312)	-0.0041(0.455)	-0.0037(0.211)
Rb-plt	-0.0173(0.375)	-0.0146(0.337)	-0.0125(0.466)	-0.0151(0.402)	-0.0188(0.316)
Sr-plt	-0.0149(0.340)	-0.0155(0.300)	-0.0126(0.273)	-0.0168(0.175)	-0.0040(0.010)
^{95}Mo-plt	-0.0163(0.175)	-0.0089(0.012)	-0.0143(0.208)	-0.0143(0.269)	-0.0111(0.102)
^{98}Mo-plt	-0.0136(0.472)	-0.0140(0.378)	-0.0083(0.072)	-0.0106(0.242)	-0.0147(0.509)
Ru-plt	0.0038(0.002)	0.0032(0.001)	-0.0035(0.214)	-0.0029(0.146)	-0.0030(0.273)
Rh-plt	-0.0018(0.140)	-0.0027(0.037)	-0.0033(0.502)	-0.0031(0.415)	-0.0036(0.250)
Pd-plt	-0.0052(0.180)	-0.0022(0.017)	-0.0049(0.386)	-0.0055(0.379)	-0.0052(0.073)
^{106}Cd-plt	-0.0234(0.326)	-0.0212(0.210)	-0.0185(0.207)	-0.0241(0.305)	0.0028(0.022)
^{111}Cd-plt	0.0179(0.001)	-0.0047(0.030)	-0.0052(0.040)	-0.0048(0.080)	-0.0101(0.442)
^{120}Sn-plt	-0.0106(0.080)	-0.0120(0.048)	-0.0105(0.022)	-0.0063(0.040)	-0.0079(0.066)
Sb-plt	-0.0075(0.278)	-0.0085(0.364)	-0.0066(0.296)	-0.0070(0.198)	-0.0088(0.447)
Te-plt	-0.0010(0.065)	-0.0015(0.046)	-0.0032(0.413)	-0.0027(0.179)	-0.0034(0.208)
Cs-plt	-0.0213(0.440)	-0.0154(0.197)	-0.0172(0.428)	-0.0193(0.409)	-0.0178(0.346)
Ba-plt	0.0000(0.007)	-0.0120(0.292)	-0.0120(0.069)	-0.0102(0.064)	-0.0144(0.410)
La-plt	0.0034(0.008)	-0.0090(0.033)	-0.0115(0.349)	-0.0069(0.103)	-0.0153(0.383)
Ce-plt	0.0095(0.005)	-0.0055(0.017)	-0.0124(0.433)	-0.0059(0.048)	-0.0137(0.366)
Pr-plt	0.0020(0.013)	-0.0091(0.036)	-0.0117(0.416)	-0.0108(0.085)	-0.0130(0.319)
Nd-plt	0.0059(0.010)	-0.0129(0.034)	-0.0132(0.258)	-0.0097(0.076)	-0.0186(0.461)
Sm-plt	-0.0089(0.053)	-0.0117(0.146)	-0.0109(0.262)	-0.0155(0.146)	-0.0139(0.304)
Eu-plt	-0.0104(0.117)	-0.0138(0.220)	-0.0111(0.163)	-0.0160(0.215)	-0.0141(0.241)
Gd-plt	0.0058(0.011)	-0.0081(0.071)	-0.0127(0.359)	-0.0057(0.055)	-0.0130(0.264)
Dy-plt	-0.0028(0.023)	-0.0137(0.094)	-0.0181(0.489)	-0.0049(0.052)	-0.0153(0.227)
Ho-plt	-0.0106(0.066)	-0.0126(0.056)	-0.0155(0.082)	-0.0085(0.054)	-0.0072(0.070)
Er-plt	-0.0025(0.049)	-0.0110(0.131)	-0.0112(0.162)	-0.0052(0.056)	-0.0128(0.236)
Tm-plt	-0.0086(0.152)	-0.0093(0.265)	-0.0096(0.213)	0.0006(0.016)	0.0096(0.003)
Yb-plt	-0.0087(0.089)	-0.0102(0.213)	-0.0107(0.138)	-0.0056(0.039)	-0.0054(0.079)
Lu-plt	-0.0091(0.368)	-0.0067(0.428)	-0.0055(0.255)	-0.0073(0.369)	-0.0076(0.518)
Hf-plt	0.0237(0.005)	-0.0170(0.454)	-0.0172(0.133)	-0.0053(0.039)	-0.0180(0.155)
Ta-plt	-0.0026(0.204)	-0.0028(0.483)	-0.0021(0.238)	-0.0024(0.239)	-0.0029(0.338)
W-plt	-0.0043(0.381)	-0.0057(0.132)	-0.0044(0.106)	-0.0040(0.129)	-0.0051(0.130)
Re-plt	0.0113(0.001)	0.0031(0.001)	-0.0024(0.491)	-0.0007(0.018)	-0.0028(0.402)
Pt-plt	-0.0165(0.464)	-0.0119(0.151)	-0.0149(0.216)	-0.0141(0.375)	-0.0152(0.269)
Tl-plt	-0.0155(0.232)	-0.0159(0.194)	-0.0176(0.442)	-0.0170(0.336)	-0.0135(0.123)
^{208}Pb-plt	-0.0169(0.346)	-0.0211(0.295)	-0.0175(0.253)	-0.0176(0.252)	-0.0153(0.235)
Th-plt	0.0035(0.005)	-0.0161(0.426)	-0.0190(0.472)	-0.0021(0.015)	-0.0160(0.267)
AODC	-0.0205(0.214)	-0.0138(0.117)	-0.0169(0.256)	-0.0191(0.412)	-0.0156(0.305)

Supplementary Table 7 The performance indexes and top 10 environmental variables of Orthogonal Partial Least Squares (OPLS) model for each assembly process. R^2_Y and R^2_X represent the percentage of Y (i.e., relative importance of assembly process) and X (i.e. environmental variables) dispersion (i.e., sum of squares) explained by the model, respectively; Q^2_Y reflects the overall predictive performance of the model; P_{Q2Y} and P_{R2Y} reflect the significance of Q^2_Y and R^2_Y compared to the results from random permutations; VIP, variable importance in projection, of which the values >1 point to the most relevant variables. Depth (T) and (B) indicate the depth of the screen top and bottom, respectively; -sup, in supernatant; -ss, in suspended solid; -plt, in pellet.

Index	**Heterogeneous Selection**		**Homogeneous Selection**		**Dispersal Limitation**		**Homogenizing Dispersal**		**'Drift'**	
Q^2_Y	0.441		0.110		0.068		0.291		0.326	
P_{Q2Y}	0.001		0.001		0.001		0.150		0.005	
R^2_Y	0.483		0.144		0.113		0.339		0.385	
P_{R2Y}	0.001		0.001		0.001		0.085		0.01	
R^2_X	0.311		0.233		0.233		0.271		0.329	
Rank	**Variable**	**VIP**	**Variable**	**VIP**	**Variable**	**VIP**	**Variable**	**VIP**	**Variable**	**VIP**
1	pH	2.41	Elevation	3.53	^{98}Mo-sup	3.14	La-sup	2.24	Sr	3.86
2	Co	2.30	Depth (B)	3.49	^{95}Mo-sup	2.96	pH	2.16	^{106}Cd-plt	2.93
3	Eu-sup	2.10	Depth (T)	3.19	^{95}Mo-ss	2.54	Co	2.15	As	2.79
4	^{98}Mo-sup	2.06	pH	3.07	^{98}Mo-ss	2.47	Co-ss	2.13	Sr-plt	2.45
5	Co-ss	2.03	CO_2	2.93	Zn	2.06	Gd-sup	2.10	Hf-ss	2.44
6	^{95}Mo-sup	2.00	Screen	2.42	Al	1.99	Ni-ss	2.07	Tm-plt	2.36
7	La-sup	1.97	SO_4^{2-}	2.39	Eu-ss	1.95	^{111}Cd-sup	1.99	CH_4	2.01
8	Ca	1.96	Mn	2.38	CO_2	1.92	SO_4^{2-}	1.95	Cu	1.94
9	Gd-sup	1.96	DOC	2.36	Nd-ss	1.87	Ca	1.88	Br^-	1.93
10	Eu-ss	1.95	Ca	2.29	Eu-sup	1.83	^{111}Cd-ss	1.84	Fe	1.91

Supplementary Table 8 The number of missing data points (m) of each environmental variable and the coefficient of determination (R^2) of the multiple linear regression model used to estimate the missing values.

No.	Category	Variable	m	R^2
1	Spatial	Coordinate (East.)	0	/
2		Coordinate (North.)	0	/
3		Elevation	0	/
4		Depth (T)	0	/
5		Depth (B)	0	/
6		Screen	0	/
7	Climate	Temperature	0	/
8	Biomass	AODC	4	0.957
9	pH	pH	0	/
10	Conductivity	Conductivity	0	/
11	DO/Redox	Redox	0	/
12		DO	0	/
13	Carbon	DIC	0	/
14		DOC	0	/
15	Gas	O_2	12	1.000
16		CH_4	12	0.912
17		CO_2	12	0.890
18		N_2	12	0.526
19		N_2O	12	0.922
20	Anion	Sulfide	0	/
21		Cl^-	0	/
22		Br^-	0	/
23		NO_3^-	0	/
24		PO_4^{3-}	0	/
25		SO_4^{2-}	0	/
26		NO_2^-	1	0.980
27	Metal (overall)	Fe (II)	0	/
28		K	1	0.912
29		Na	1	0.925
30		Ca	1	0.953
31		Mg	1	0.941
32		Al	10	0.936
33		Ba	1	0.993
34		Ag	1	0.974
35		As	1	0.972
36		Be	1	0.996
37		Bi	1	1.000
38		Cd	1	0.991
39	Metal (overall	Co	1	0.999
40		Cr	1	0.984
41		Cs	1	1.000
42		Cu	1	0.991
43		Zn	1	0.996
44		Fe	1	0.981
45		Ga	1	0.991
46		Mn	1	0.982
47		Li	1	0.980
48		Ni	1	0.980
49		Pb	1	0.980
50		Se	1	0.980
51		Sr	1	0.979
52		U	1	0.983
53	Metal in supernatant	U-sup	1	0.998
54		Ti-sup	1	0.999
55		V-sup	1	0.998
56		^{52}Cr-sup	1	1.000
57		^{53}Cr-sup	1	1.000
58		Mn-sup	1	1.000
59		Fe-sup	1	1.000
60		Co-sup	1	1.000
61		Ni-sup	1	1.000
62		Cu-sup	1	1.000
63		^{66}Zn-sup	1	1.000
64		^{68}Zn-sup	1	1.000
65		Ga-sup	1	1.000
66		Ge-sup	1	1.000
67		As-sup	1	1.000
68		Rb-sup	1	1.000
69		Sr-sup	1	1.000
70		^{95}Mo-sup	1	1.000
71		^{98}Mo-sup	1	1.000
72		Ru-sup	1	1.000
73		Rh-sup	1	1.000
74		Pd-sup	1	1.000
75		^{106}Cd-sup	1	1.000
76		^{111}Cd-sup	1	1.000

Supplementary Table 8 (Continued)

No.	Category	Variable	m	R^2
77	Metal in supernatant	^{120}Sn-sup	1	1.000
78		Sb-sup	1	1.000
79		Te-sup	1	1.000
80		Cs-sup	1	1.000
81		Ba-sup	1	1.000
82		La-sup	1	1.000
83		Ce-sup	1	1.000
84		Pr-sup	1	1.000
85		Nd-sup	1	1.000
86		Sm-sup	1	1.000
87		Eu-sup	1	1.000
88		Gd-sup	1	1.000
89		Dy-sup	1	1.000
90		Ho-sup	1	1.000
91		Er-sup	1	1.000
92		Tm-sup	1	1.000
93		Yb-sup	1	0.999
94		Lu-sup	1	1.000
95		Hf-sup	1	0.999
96		Ta-sup	1	0.999
97		W-sup	1	0.999
98		Re-sup	1	0.999
99		Pt-sup	1	0.999
100		Tl-sup	1	0.999
101		^{208}Pb-sup	1	0.999
102		Th-sup	1	1.000
103	Metal in suspended solid	U-ss	1	0.999
104		Ti-ss	1	1.000
105		V-ss	1	0.999
106		^{52}Cr-ss	1	0.999
107		^{53}Cr-ss	1	1.000
108		Mn-ss	1	1.000
109		Fe-ss	1	1.000
110		Co-ss	1	1.000
111		Ni-ss	1	1.000
112		Cu-ss	1	1.000
113		^{66}Zn-ss	1	1.000
114		^{68}Zn-ss	1	1.000
115		Ga-ss	1	1.000
116		Ge-ss	1	0.999
117		As-ss	1	0.999
118		Rb-ss	1	1.000

No.	Category	Variable	m	R^2
119	Metal in suspended solid	Sr-ss	1	1.000
120		^{95}Mo-ss	1	1.000
121		^{98}Mo-ss	1	1.000
122		Ru-ss	1	0.999
123		Rh-ss	1	1.000
124		Pd-ss	1	0.999
125		^{106}Cd-ss	1	1.000
126		^{111}Cd-ss	1	0.999
127		^{120}Sn-ss	1	0.999
128		Sb-ss	1	0.999
129		Te-ss	1	0.998
130		Cs-ss	1	1.000
131		Ba-ss	1	1.000
132		La-ss	1	1.000
133		Ce-ss	1	0.999
134		Pr-ss	1	0.997
135		Nd-ss	1	1.000
136		Sm-ss	1	1.000
137		Eu-ss	1	1.000
138		Gd-ss	1	1.000
139		Dy-ss	1	1.000
140		Ho-ss	1	1.000
141		Er-ss	1	1.000
142		Tm-ss	1	0.999
143		Yb-ss	1	1.000
144		Lu-ss	1	1.000
145		Hf-ss	1	1.000
146		Ta-ss	1	1.000
147		W-ss	1	1.000
148		Re-ss	1	1.000
149		Pt-ss	1	1.000
150		Tl-ss	1	0.998
151		^{208}Pb-ss	1	0.998
152		Th-ss	1	1.000
153	Metal in pellet	U-plt	1	1.000
154		Ti-plt	1	1.000
155		V-plt	1	1.000
156		^{52}Cr-plt	1	1.000
157		^{53}Cr-plt	1	1.000
158		Mn-plt	1	1.000
159		Fe-plt	1	0.997
160		Co-plt	1	1.000

Supplementary Table 8 (Continued)

No.	Category	Variable	m	R^2
161	Metal in pellet	Ni-plt	1	1.000
162		Cu-plt	1	1.000
163		^{66}Zn-plt	1	1.000
164		^{68}Zn-plt	1	1.000
165		Ga-plt	1	0.999
166		Ge-plt	1	0.999
167		As-plt	1	1.000
168		Rb-plt	1	0.995
169		Sr-plt	1	0.989
170		^{95}Mo-plt	1	0.981
171		^{98}Mo-plt	1	0.984
172		Ru-plt	1	1.000
173		Rh-plt	1	1.000
174		Pd-plt	1	1.000
175		^{106}Cd-plt	1	1.000
176		^{111}Cd-plt	1	1.000
177		^{120}Sn-plt	1	1.000
178		Sb-plt	1	1.000
179		Te-plt	1	1.000
180		Cs-plt	1	0.999
181		Ba-plt	1	0.993
182	Metal in pellet	La-plt	1	1.000
183		Ce-plt	1	1.000
184		Pr-plt	1	0.999
185		Nd-plt	1	0.972
186		Sm-plt	1	0.964
187		Eu-plt	1	1.000
188		Gd-plt	1	1.000
189		Dy-plt	1	0.992
190		Ho-plt	1	1.000
191		Er-plt	1	1.000
192		Tm-plt	1	1.000
193		Yb-plt	1	1.000
194		Lu-plt	1	1.000
195		Hf-plt	1	1.000
196		Ta-plt	1	1.000
197		W-plt	1	0.993
198		Re-plt	1	0.976
199		Pt-plt	1	0.970
200		Tl-plt	1	1.000
201		^{208}Pb-plt	1	1.000
202		Th-plt	1	0.951

Supplementary Table 9 The taxonomic information of reference taxa. The reference taxa were defined as taxa with mean relative abundance > 0.1% and occurrence frequency > 50% in ‘uncontaminated’ samples where no stress indicator showed a higher concentration than the reference level.

OTUID	Phylum	Class	Order	Family	Genus
744404	Myxococcota	bacteriap25	bacteriap25	bacteriap25	bacteriap25
814489	WPS-2	WPS-2	WPS-2	WPS-2	WPS-2
1062748	Actinobacteriota	Actinobacteria	Corynebacteriales	Mycobacteriaceae	Mycobacterium
1081815	Actinobacteriota	Actinobacteria	Micrococcales	Micrococcaceae	Unclassified
104069	Bacteroidota	Bacteroidia	Chitinophagales	Chitinophagaceae	Asinibacterium
781203	Bacteroidota	Bacteroidia	Chitinophagales	Chitinophagaceae	Sediminibacterium
1087471	Bacteroidota	Bacteroidia	Sphingobacteriales	env.OPS_17	env.OPS_17
371510	Bacteroidota	Bacteroidia	Sphingobacteriales	Sphingobacteriaceae	Pedobacter
142598	Nitrospirota	Nitrospiria	Nitrospirales	Nitrospiraceae	Nitrospira
808092	Nitrospirota	Nitrospiria	Nitrospirales	Nitrospiraceae	Nitrospira
328951	Nitrospirota	Nitrospiria	Nitrospirales	Nitrospiraceae	Nitrospira
537655	Nitrospirota	Nitrospiria	Nitrospirales	Nitrospiraceae	Nitrospira
2760486	Elusimicrobiota	Elusimicrobia	Lineage_IV	Lineage_IV	Lineage_IV
606431	Elusimicrobiota	Elusimicrobia	Lineage_IV	Lineage_IV	Lineage_IV
New.ReferenceOTU116424	Proteobacteria	Alphaproteobacteria	uncultured	uncultured	uncultured
674655	Proteobacteria	Alphaproteobacteria	Sphingomonadales	Sphingomonadaceae	Sphingopyxis
813418	Proteobacteria	Alphaproteobacteria	Sphingomonadales	Sphingomonadaceae	Novosphingobium
222183	Proteobacteria	Alphaproteobacteria	Sphingomonadales	Sphingomonadaceae	Sphingomonas
1003206	Proteobacteria	Alphaproteobacteria	Sphingomonadales	Sphingomonadaceae	Sphingomonas
818854	Proteobacteria	Alphaproteobacteria	Rhodobacterales	Rhodobacteraceae	Rhodobacter
568617	Proteobacteria	Alphaproteobacteria	Reyranellales	Reyranellaceae	Reyranella
1640195	Proteobacteria	Alphaproteobacteria	Reyranellales	Reyranellaceae	Reyranella
709657	Proteobacteria	Alphaproteobacteria	Reyranellales	Reyranellaceae	Reyranella
969805	Proteobacteria	Alphaproteobacteria	Rhizobiales	Rhizobiaceae	Allorhizobium-Neorhizobium-

OTUID	Phylum	Class	Order	Family	Genus
					Pararhizobium-Rhizobium
841170	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Brevundimonas
998905	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Brevundimonas
248395	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Caulobacter
541299	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Caulobacter
811449	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Caulobacter
209762	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Phenylobacterium
574416	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Unclassified
46818	Proteobacteria	Alphaproteobacteria	Caulobacterales	Caulobacteraceae	Phenylobacterium
567336	Proteobacteria	Alphaproteobacteria	Rhizobiales	Beijerinckiaceae	Bosea
574655	Proteobacteria	Alphaproteobacteria	Rhizobiales	Beijerinckiaceae	Methylobacterium-Methylorubrum
580625	Proteobacteria	Alphaproteobacteria	Rhizobiales	Xanthobacteraceae	Unclassified
567840	Proteobacteria	Alphaproteobacteria	Rhizobiales	Xanthobacteraceae	Unclassified
934235	Proteobacteria	Alphaproteobacteria	Rhizobiales	Beijerinckiaceae	Unclassified
583489	Proteobacteria	Gammaproteobacteria	Burkholderiales	TRA3-20	TRA3-20
961783	Proteobacteria	Gammaproteobacteria	Pseudomonadales	Pseudomonadaceae	Pseudomonas
646549	Proteobacteria	Gammaproteobacteria	Pseudomonadales	Pseudomonadaceae	Pseudomonas
974121	Proteobacteria	Gammaproteobacteria	Pseudomonadales	Pseudomonadaceae	Pseudomonas
982582	Proteobacteria	Gammaproteobacteria	Xanthomonadales	Xanthomonadaceae	Lysobacter
225453	Proteobacteria	Gammaproteobacteria	Cellvibrionales	Cellvibrionaceae	Cellvibrio
4478803	Proteobacteria	Gammaproteobacteria	Salinisphaerales	Solimonadaceae	uncultured
1116070	Proteobacteria	Gammaproteobacteria	Acidiferrobacterales	Acidiferrobacteraceae	Sulfurifustis
New.ReferenceOTU120557	Proteobacteria	Gammaproteobacteria	Acidiferrobacterales	Acidiferrobacteraceae	Sulfurifustis
813906	Proteobacteria	Gammaproteobacteria	Burkholderiales	Gallionellaceae	Sideroxydans
536398	Proteobacteria	Gammaproteobacteria	Burkholderiales	Gallionellaceae	Sideroxydans
580571	Proteobacteria	Gammaproteobacteria	Burkholderiales	Burkholderiaceae	Cupriavidus

OTUID	**Phylum**	**Class**	**Order**	**Family**	**Genus**
1118109	Proteobacteria	Gammaproteobacteria	Burkholderiales	Nitrosomonadaceae	MND1
694781	Proteobacteria	Gammaproteobacteria	Burkholderiales	Nitrosomonadaceae	MND1
1501738	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Sulfuritalea
New.ReferenceOTU27587	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Sulfuritalea
586230	Proteobacteria	Gammaproteobacteria	Burkholderiales	Oxalobacteraceae	Unclassified
566578	Proteobacteria	Gammaproteobacteria	Burkholderiales	Oxalobacteraceae	Unclassified
822419	Proteobacteria	Gammaproteobacteria	Burkholderiales	Oxalobacteraceae	Massilia
832674	Proteobacteria	Gammaproteobacteria	Burkholderiales	Oxalobacteraceae	Janthinobacterium
352419	Proteobacteria	Gammaproteobacteria	Burkholderiales	Gallionellaceae	Sideroxydans
531901	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Unclassified
369022	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Unclassified
738779	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Unclassified
530591	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Unclassified
745157	Proteobacteria	Gammaproteobacteria	Burkholderiales	Rhodocyclaceae	Unclassified
532139	Proteobacteria	Gammaproteobacteria	Burkholderiales	Nitrosomonadaceae	MND1
816229	Proteobacteria	Gammaproteobacteria	Burkholderiales	Nitrosomonadaceae	GOUTA6
1108275	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified
225259	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Comamonas
1108726	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified
942852	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Rhizobacter
1106617	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified
1048878	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Variovorax
719367	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified
940737	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Unclassified
815406	Proteobacteria	Gammaproteobacteria	Burkholderiales	Comamonadaceae	Hydrogenophaga
714231	Proteobacteria	Gammaproteobacteria	Xanthomonadales	Rhodanobacteraceae	Rhodanobacter