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Systematic Study on the Interaction Mechanism of Microbial Community Structure and Function

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Abstract: In diverse natural and engineered ecosystems, microbial communities play a pivotal role in material cycling and energy conversion. The interplay between community structural characteristics and functional expression is emerging as a critical pathway to understanding system homeostasis and predictability. While existing research has accumulated substantial data on diversity metrics, community assembly processes, interspecies interaction networks, and multi-omics functional analysis, efforts to integrate structural information with functional outputs across scales and establish a unified framework for interaction mechanisms remain fragmented. This study adopts a "structural analysis-interaction network-dynamic regulation and system modeling" approach. Building upon the elucidation of core structural attributes and assembly drivers, it systematically examines the relationships between interspecies interaction types, network topologies, and functional correlations. By incorporating the logic of structural plasticity and functional redundancy maintenance, along with multi-scale modeling strategies, the research explores the ecological consequences of structural-functional dysregulation and potential remediation pathways. The findings aim to provide transferable theoretical and methodological support for predictive understanding and rational regulation of microbial communities.

Keywords: Microbial community structure; Functional redundancy; Interaction network modeling

Microbial communities permeate nearly all ecological niches, ranging from aquatic environments and sediments to host-associated ecosystems and various reactor systems. Biogeochemical processes at different scales often rely on the co-evolution of community structure and function. Diversity, phylogenetic relationships, and spatial patterns form the structural framework, while metabolic pathways and ecological processes manifest as comprehensive effects such as gas fluxes, nutrient transformation, and signal regulation on the functional side. Existing research indicates that subtle adjustments in community structure can trigger nonlinear responses in functional output and robustness, making structure-function coupling a critical tool for predicting system behavior [1]. With the maturation of high-throughput omics and network analysis tools, extracting interpretable interaction mechanisms from multidimensional structural features, interspecies interaction

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networks, and assembly process information, and providing testable predictions at the dynamic and system modeling levels, has become a key challenge for microbial ecology and engineering microbiology.

1 Multidimensional Analysis of Microbial Community Structure

1.1 Core Attributes and Quantitative Indicators of Community Structure

Microbial community structure is typically characterized through three dimensions: diversity, compositional structure, and phylogenetic relationships. Diversity indices and abundance distributions reflect species richness and evenness, while phylogenetic metrics reveal the degree of phylogenetic clustering or divergence. Researchers also distinguish core communities that consistently emerge across multiple samples from rare taxa in the long tail, thereby capturing both stable functional baselines and potential stress response reserves. With the integration of network perspectives, topological indicators such as node degree, modularization, and clustering coefficients have been incorporated into the structural characterization framework. This transformation transforms microbial communities from mere species lists into interconnected relational networks with hierarchical relationships.

1.2 Driving Factors and Structural Plasticity of Community Assembly

The formation of community structure results from the combined effects of environmental selection, interspecific interactions, and stochastic processes. Environmental filtering determines which taxa have long-term persistence potential based on resource availability and physicochemical conditions, while diffusion constraints and genetic drift introduce historical path differences. Decomposition analyses using empty models and neutral models reveal significant variations in the contribution ratios of directed and stochastic processes to assembly patterns across different ecosystems, indicating that assembly mechanisms are closely linked to structural plasticity [2]. When external disturbances alter environmental conditions or diffusion patterns, communities often undergo reorganization in species composition, relative abundance, and interactions. This plasticity not only provides space for functional redundancy but also creates structural buffer zones for subsequent intervention strategies.

2 Construction and Functional Regulation of Two Species Interactions Networks

2.1 Main Types and Molecular Basis of Interspecific Interaction

Within microbial communities, species engage in diverse interactions—including competition, mutualism, commensalism, and antagonism—through resource utilization and metabolic complementarity. These interactions are underpinned by molecular mechanisms such as metabolic product exchange, signaling molecule transmission, and the secretion of inhibitory substances. Mutualistic interactions typically occur in metabolic cascades, where one microbial group breaks down complex substrates into intermediate products, which are then further metabolized by another group, thereby optimizing energy utilization at the population level. Competitive interactions, on the other hand, revolve around limiting resources and are often accompanied by the release of inhibitors or toxins. Research has introduced the concept of "key taxa," identifying species that serve as hubs connecting multiple interaction pathways within the network. Their metabolic characteristics and regulatory capabilities can amplify the overall functional stability and robustness of the community [3].

2.2 Topological Features and Functional Relevance of Interactive Networks

Using high-throughput sequencing data and statistical inference methods, researchers constructed species-based interaction networks with species as nodes and cooperative or antagonistic relationships as edges. Degree distribution, median centrality, and modular structure became key perspectives for identifying potential hub species and functional modules. The degree of network modularization is often correlated with a system's ability to isolate disturbances. Moderate modularization helps establish a buffer zone between local changes and overall homeostasis, while highly central nodes across modules may serve functions such as functional coupling and cross-scale signal transmission. Functional correlation analysis typically links process rates, metabolic fluxes, or phenotypic indicators with network topological features, examining whether high-connectivity regions are enriched with specific functional pathways or whether the removal of key nodes triggers functional collapse. These results indirectly support the logic of "structure-limiting functional space."

2.3 Regulatory Effects of Environmental Factors on Interaction Networks

Environmental factors shape interactive networks through dual mechanisms: altering resource and energy input patterns while reconstructing spatial structures and diffusion pathways. Physicochemical variables including nutrient levels, redox states, and pH modify the relative fitness of species, thereby adjusting competitive and symbiotic relationships to rebalance network edge weights and connectivity. Spatial heterogeneity and microenvironmental structures influence the stability of localized interaction clusters, where micro-scale isolation mitigates intense competition and enhances the durability of synergistic metabolic pathways. Persistent disturbances or continuous gradients often drive network transitions between topological configurations, manifesting as module boundary remodeling, hub species replacement, and key pathway reorganization, profoundly impacting functional robustness and adaptability.

3 Dynamic Regulation and System Modeling of Structure-Function Interactions

3.1 Synergistic Maintenance Mechanism of Structural Plasticity and Functional Redundancy

From a long-term evolutionary perspective, microbial communities often develop a coordinated configuration between structural plasticity and functional redundancy to cope with multi-source disturbances and resource fluctuations. Structural plasticity manifests as the ability of species combinations and interactions to reconfigure after disturbances, allowing newly introduced or previously rare taxa to gain growth opportunities when environmental conditions change, while dominant taxa gradually exit under unfavorable conditions. Functional redundancy refers to multiple species sharing similar metabolic capabilities or ecological roles, enabling other species to compensate for local population damage and maintain continuity of critical processes in the short term [4].

Time series and disturbance experiments often reveal a dynamic pattern of "rapid functional recovery—slow structural convergence." Functional metrics quickly return to near-initial levels after disturbances are removed, while species composition and network topology undergo gradual adjustments over longer time scales. Redundancy is not always advantageous; excessive redundancy may reduce system efficiency under resource constraints, whereas insufficient redundancy makes the system highly susceptible to functional collapse when facing new disturbances. Structural plasticity acts as a regulator, allowing the specific bearers of redundancy and interaction pathways to be reallocated based on environmental states. Together, these mechanisms form a "robust yet flexible" structure-function maintenance mechanism.

3.2 Multiscale Modeling Approach for Structure-Function Interaction

To characterize the dynamic process of structure-function interactions at the system level, researchers have progressively developed a cross-scale modeling framework that integrates species abundance, interaction networks, and metabolic flux pathways into a unified logical system. The ecological dynamics model uses species abundance as a state variable and presents the combined effects of competition and mutualism through an interaction coefficient matrix, facilitating analysis of how structural perturbations influence overall functional output and steady-state positions. Meanwhile, the metabolic network and constraint optimization model focuses on the functional side, leveraging genomic annotations to construct pathway structures and predict metabolic flux allocation and resource utilization efficiency under given environmental conditions.

With the advancement of multi-omics technologies, multi-scale models integrating community composition, functional genes, transcriptomes, and metabolomes have emerged. These models typically combine machine learning with Bayesian inference to extract the most explanatory feature combinations from high-dimensional data for structure-function mapping [5]. The modeling process is no longer viewed as a unidirectional fit but emphasizes a cyclical approach between "data interpretation—mechanistic hypothesis—model prediction—experimental validation": on one hand, using observational data to calibrate model parameters and structures; on the other hand, enabling models to provide testable perturbation responses and repair pathway predictions, thereby guiding subsequent experimental design and engineering optimization. This approach advances structure-function interaction research toward a quantitative, predictable, and designable direction. Based on this, the model itself will also transform into a "navigator" for identifying key groups and functional pathways, guiding the management of the community towards more refined strategy combinations.

3.3 Ecological Consequences and Restoration Strategies of Structural-Functional Disruption

When environmental shocks or human interventions exceed a system's buffering capacity, structural-functional interactions may become disrupted. This manifests through multidimensional changes including loss of key taxa, collapse of mutualistic networks, and disruption of functional pathways, leading the system into a metastable state characterized by reduced functionality or heightened volatility. In such states, communities struggle to spontaneously return to their original steady state even when external pressures diminish, exhibiting phenomena known as "ecological memory" and "lag effects." These phenomena reflect significant temporal inertia in structural adjustments and interactive reconstruction. Functional consequences include reduced cycling rates of critical substances, diminished pollutant removal capacity, or disruption of host physiological homeostasis. Over the long term, these changes may also alter subsequent species invasion and succession trajectories.

Repair strategies for dysregulated states typically address both structural and functional dimensions. On one hand, they rely on species supplementation and reintroduction of key taxa to reshape community structures, restoring moderate diversity and rational network modularization. On the other hand, they integrate resource allocation and environmental regulation to create ecological niches conducive to the recovery of target functional pathways, enabling functionally relevant taxa to gain growth advantages. Advanced strategies tend to construct synthetic communities with clear functional orientations, complemented by exogenous substrate and operational parameter design, to guide target systems along anticipated structure-function trajectories. If repair practices can form feedback loops with the aforementioned modeling frameworks, it is expected to transition from empirical interventions to refined design under controllable risks.During this process, continuous monitoring and feedback assessment are indispensable. The intervention effects, system resilience and potential side effects need to be quantified simultaneously. Gradually accumulate reusable parameter combinations and situational cases to provide comparable and transferable decision-making basis for community restoration under different ecological niches, and lay the foundation for subsequent structural-functional synergy optimization.

4 Conclusion

The discussion on the core issue of microbial community structure-function interactions reveals that structure is not a static background but a dynamic framework evolving through assembly processes, interspecies interactions, and environmental regulation. Function, in turn, reversely shapes structural boundaries through redundant configurations and feedback regulation. The assembly mechanisms of communities, interaction network topologies, and structural plasticity collectively determine the system's response patterns under perturbations. Functional redundancy and multi-scale modeling provide support for understanding and predicting such responses. Looking ahead, establishing a tightly integrated framework linking multi-omics data, time-series observations, and controlled intervention experiments could lead to the development of a transferable structure-function interaction theory across ecosystems. This would lay a more solid theoretical foundation for microbial community management in environmental governance, engineering process optimization, and host health interventions.

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