

Suggested Topics for AI-Agents 2025 Conference

Suggested topics include but are not restricted to the following:

Molecule AI Agents

- **Protein structure prediction**
 - Prediction of protein folding patterns and three-dimensional structures from sequence data
 - Simulate changes in protein conformation
- **Molecular docking**
 - Prediction of protein-protein interactions
 - Prediction of protein complexes and structures
 - Prediction of protein and small molecule binding
 - Prediction of and nucleic acid binding
 - Prediction of the docking molecules based on protein conformation
- **Post-translation modification analysis**
 - Prediction of post-translational modification sites
 - Simulate and predict the effects of PTM on protein structure, function, and stability
 - Design precision therapeutic drugs targeting the PTM pathway
- **Protein functional annotation**
 - Annotations on the functional domains of proteins
 - Classification of protein families
 - Prediction of enzyme activity
 - Prediction of binding affinity and catalytic residues
 - Prediction of changes in protein function caused by gene mutations
- **Protein design and engineering**
 - Design proteins with specific functions
 - Prediction of and optimization of gene sequences based on protein conformation
 - Designing proteins from scratch to optimize enzyme activity

Organelle AI Agents

- **Mitochondrial cell-dependent properties**
 - Mitochondrial function prediction
 - Mitochondrial morphology and distribution prediction
 - Mitochondrial lineage prediction
 - Mitochondrial heterogeneity prediction
 - Mitochondrial transfer prediction

- **Mitochondrial molecular features**

- mtDNA variation detection
- Mitochondrial mutation pathogenicity prediction
- Mitochondrial protein structure prediction
- Drug effects prediction
- Drug targets identification

- **Mitochondrial activities**

- Mitochondrial Energy metabolism prediction
- Mitochondrial membrane components prediction
- Neuronal activity prediction
- Cell apoptosis prediction

- **Mitochondrial functions**

- Efficiency of mitochondrial ATP generation prediction
- Mitochondrial calcium ion concentration prediction
- mtROS levels prediction
- Multi omics data mining and functional modeling

- **Mitochondrial behaviors**

- Mitochondrial fusion and fission dynamics identification
- Mitochondrial movement patterns prediction
- Impact of mitochondrial signaling on nuclear gene expression prediction
- Interaction between mitochondria and nucleus prediction

Cell AI Agents

- **Cell function**

- Construction of intracellular metabolic network
- The functional adjustments of cells under environmental changes prediction
- Prediction of the association between cells and diseases

- **Cell behaviors**

- Cell migration prediction
- Cell cycle prediction
- Cell differentiation prediction
- Cell apoptosis and autophagy prediction
- Inferring the spatial distribution and composition of cells

- **Cell molecular features**

- Cell gene expression prediction
- Prediction of regulatory relationships between genes

- Cell variation detection
- Cell non-genetic variation detection
- Cell mutation pathogenicity prediction
- Cell protein structure prediction
- **Cellular heterogeneity**
 - Cell classification and functional prediction
 - Prediction of gene expression in different life cycles of cells
 - Prediction of cellular functional subtypes
 - Cell trajectory inference
- **Cellular interactions**
 - Cross-cell signal prediction
 - Prediction of the interaction between cells and cell-matrix
 - Prediction of molecular changes in intercellular interactions
 - Inferring ligand-receptor interactions between cells
- **Cellular diagnosis and therapy**
 - Discovery of disease biomarkers
 - Prediction of drug reactions in cells
 - Optimization of cellular molecules
 - Cell therapy optimization
 - Disease prediction
 - Immune escape prediction

Tissue AI Agents

- **Tissue function**
 - Simulate functional dynamics within an organization
 - Predicting the impact of different environments on organizational function
- **Tissue behaviors**
 - Prediction of the dynamic behavior of an organization
 - Prediction of cell migration, proliferation, and apoptosis within tissues
- **Tissue molecular features**
 - Identify tissue-specific molecular markers
 - Prediction of molecular changes in organizations
- **Tissue heterogeneity**

- Prediction of heterogeneity in different regions of an organization, including cell types, metabolic activity, and molecular distribution
- Prediction of the spatial stratification and distribution of organizational functions

- **Tissue diagnosis and therapy**

- Prediction of drug response to specific tissues
- Optimizing tissue engineering and regenerative medicine solutions

Organ AI Agents

- **Organ function modeling**

- Simulate and predict the functional status of a single organ under healthy and diseased conditions
- Simulate and predict the impact of the environment on organ function

- **Organ pathophysiology analysis**

- Dynamic changes of simulator-specific diseases
- Prediction of the causes of organ dysfunction

- **Organ molecular features**

- Identifying organ-specific marker genes
- Molecular characteristics under pathological progression prediction

- **Organ heterogeneity**

- Prediction of heterogeneity in different regions of an organization, including cell types, metabolic activity, and molecular distribution
- Prediction of the spatial stratification and distribution of organizational functions

- **Tissue interactions**

- Building a communication network between organizations
- Simulate signal transmission between organizations

- **Drug response and toxicity analysis**

- Prediction of the effects of drugs on specific organs
- Optimizing organ engineering and regenerative medicine solutions
- Simulating the adaptation process of transplanted organs in the host

Organ System AI Agents

- **Multi-organ functional coordination**

- Building functionally related networks for multiple organs
- Prediction of how multiple organ dysfunction can lead to systemic diseases
- **Multi-organ signal transmission and regulation**
 - Prediction of the propagation path of cellular signals between multiple organs
 - Analyzing how the signal imbalance between organs triggers pathological cascade effects
- **Multi-organ pathological cascades**
 - Simulate the dynamic process of disease spreading from one organ to other organs
- **Multi-organ damage and repair**
 - Simulating the process of cross-organ compensation and repair after organ injury
- **Multi-organ metabolic networks**
 - Constructing a metabolic flow and balance network among multiple organs
 - Prediction of the flow and changes of metabolites in multiple organs
- **Multi-organ biomechanical interactions**
 - Analyze the impact of inter-organ interactions on functional performance
 - Prediction of phenotype-related organs and organ changes
- **Multi-organ responses and adaptations of drugs**
 - Optimize multi-organ treatment plan
 - Prediction of the multi-organ combined effects of drugs

Body AI Agents

- **Intra-system functional coordination**
 - Prediction of the functional within the system
 - Building a functional dynamic model of multiple organs within the system
- **Inter-system functional coupling**
 - Simulate the functional coupling and mutual adjustment between different systems
 - Prediction of how neural signals propagate between the nervous system and musculoskeletal system
- **System-level signal transmission and regulation**
 - Simulate the dynamic process of disease spreading from one organ to other organs
- **Systemic disease propagation**
 - Simulate the dynamic transmission of diseases within and between systems

- **System-level metabolic dynamics**

- Constructing metabolic flow pathways within and between systems
- Prediction of how lipid metabolism disorders affect systemic energy balance through the digestive and circulatory systems

- **Mechanics and structural interactions**

- Simulate the impact of internal and external mechanical interactions on system functionality

- **Personalized system-level therapy optimization**

- Simulate the combined effects of drugs on multiple systems and optimize therapies
- Design anti-cancer drugs that target the immune system while protecting the functions of the circulatory and digestive systems