Suggested Topics for AI-AGENT 2025 Conference

Suggested topics including but not restricted to the following:

Molecule AI Agent

- **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 optimizing gene sequences based on protein conformation
    -Designing proteins from scratch to optimize enzyme activity

Organelle AI Agent

- **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 Agent

- **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 Agent

- **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 Agent

- **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 Agent

- **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 Agent

- **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