

## **Suggested Topics for AAIC 2026 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