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AI-Driven Metabolmics for Precision Nutrition: Tailoring Dietary Recommendations based on Individual Health Profiles.

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Abstract: - Precision nutrition represents a transformative approach to dietary recommendations, aiming to tailor nutritional interventions to individual characteristics, including genetics, lifestyle, and health status. Metabolomics, the systematic study of small molecules or metabolites in biological systems, offers a comprehensive framework for assessing an individual's metabolic profile and response to dietary interventions. By integrating advanced analytics techniques with metabolomics data, artificial intelligence (AI) enables the development of personalized dietary recommendations based on individual health profiles. This abstract explores the potential of AI-driven metabolomics in precision nutrition, focusing on its applications, challenges, and implications for public health. Metabolomics provides a holistic view of an individual's metabolic status, capturing the dynamic interplay between diet, metabolism, and health. By profiling metabolites in biofluids, tissues, or microbiota, metabolomics offers insights into nutrient metabolism, metabolic pathways, and physiological responses to dietary intake. Recent advances in analytical techniques, such as mass spectrometry and nuclear magnetic resonance spectroscopy, have expanded the scope and resolution of metabolomics studies, facilitating the integration of metabolomics data with other omics datasets for comprehensive molecular phenotyping. AI-driven approaches, including machine learning and deep learning, offer powerful tools for analyzing complex metabolomics data and extracting meaningful insights. Machine learning algorithms can be applied to classify samples, identify biomarkers, and predict metabolic phenotypes based on metabolomics data. Deep learning models enable feature learning, dimensionality reduction, and pattern recognition in high-dimensional metabolomics datasets. By leveraging AI-driven approaches, researchers can uncover hidden patterns, associations, and interactions within metabolomics data, enabling the development of personalized dietary recommendations tailored to individual health profiles. Despite the promise of AI-driven metabolomics in precision nutrition, several challenges need to be addressed to realize its full potential. These include data integration, model interpretability, validation, and translation into clinical practice. Integrating metabolomics data with other omics datasets and clinical outcomes requires standardized data preprocessing, feature selection, and model evaluation procedures. Interpreting AI-driven models and translating findings into actionable dietary recommendations necessitates interdisciplinary collaboration between nutritionists, bioinformaticians, and data scientists. AI-driven metabolomics holds tremendous promise for advancing precision nutrition research and practice. By integrating advanced analytics techniques with metabolomics data, researchers can develop personalized dietary recommendations tailored to individual health profiles, ultimately empowering individuals to make informed dietary choices and achieve optimal health outcomes.

Keywords: - Precision nutrition, Metabolomics, Artificial intelligence, Personalized dietary recommendations, Individual health profiles, Biomarker discovery, Machine learning, Health optimization**.**

A.Introduction: Precision nutrition represents a paradigm shift in the field of dietary recommendations, moving away from generic guidelines towards personalized interventions tailored to individual characteristics. With the rise of chronic diseases and the growing recognition of the role of diet in health outcomes, there is increasing interest in leveraging advanced technologies to develop personalized dietary strategies that optimize health and well-being. Metabolomics, as a key omics technology, offers a powerful approach to characterizing an individual's metabolic profile and understanding how dietary interventions influence metabolism and health. By combining metabolomics with artificial intelligence (AI) techniques, such as machine learning and deep learning, it is possible to uncover complex relationships between dietary intake, metabolic pathways, and health outcomes. The aim of this paper is to explore the potential of AI-driven metabolomics for precision nutrition, focusing on the development of personalized dietary recommendations based on individual health profiles. We will discuss the applications, challenges, and implications of AI-driven metabolomics in precision nutrition, highlighting recent advances and emerging trends in the field. Metabolomics involves the systematic analysis of small molecules or metabolites in biological samples, providing a comprehensive snapshot of an individual's metabolic status. By profiling metabolites in biofluids, tissues, or microbiota, metabolomics enables researchers to identify biomarkers of dietary intake, nutrient metabolism, and disease risk. Recent advances in analytical techniques, such as mass spectrometry and nuclear magnetic resonance spectroscopy, have expanded the scope and resolution of metabolomics studies, facilitating the integration of metabolomics data with other omics datasets for comprehensive molecular phenotyping.

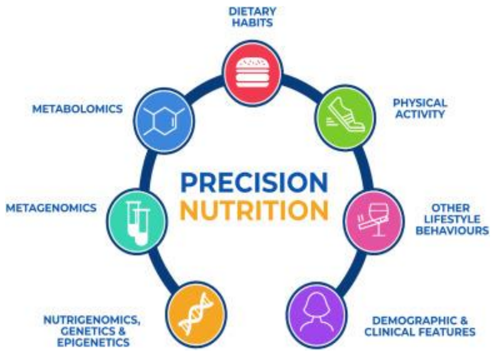

Figure 1 Precision Nutrition for Individuals.

AI-driven approaches offer powerful tools for analyzing complex metabolomics data and extracting meaningful insights. Machine learning algorithms can be applied to classify samples, identify biomarkers, and predict metabolic phenotypes based on metabolomics data. Deep learning models enable feature learning, dimensionality reduction, and pattern recognition in high-dimensional metabolomics datasets. By leveraging AI-driven approaches, researchers can uncover hidden patterns, associations, and interactions within metabolomics data, enabling the development of personalized dietary recommendations tailored to individual health profiles. Despite the promise of AI-driven metabolomics in precision nutrition, several challenges need to be addressed to realize its full potential. These include data integration, model interpretability, validation, and translation into clinical practice. Integrating metabolomics data with other omics datasets and clinical outcomes requires standardized data preprocessing, feature selection, and model evaluation procedures. Interpreting AI-driven models and translating findings into actionable dietary recommendations necessitates interdisciplinary collaboration between nutritionists, bioinformaticians, and data scientists. AI-driven metabolomics holds tremendous promise for advancing precision nutrition research and practice. By integrating advanced analytics techniques with metabolomics data, researchers can develop personalized dietary recommendations tailored to individual health profiles, ultimately empowering individuals to make informed dietary choices and achieve optimal health outcomes.

B.Literature Review: - The literature on AI-driven metabolomics for precision nutrition highlights the potential of integrating advanced analytics techniques with metabolomics data to develop personalized dietary recommendations tailored to individual health profiles. Several studies have demonstrated the effectiveness of this approach in uncovering complex relationships between dietary intake, metabolic pathways, and health outcomes. Metabolomics offers a comprehensive framework for assessing an individual's metabolic profile and understanding how dietary interventions influence metabolism and health. By profiling metabolites in biological samples, metabolomics enables researchers to identify biomarkers of dietary intake, nutrient metabolism, and disease risk. Recent advancements in analytical techniques, such as mass spectrometry and nuclear magnetic resonance spectroscopy, have enhanced the resolution and sensitivity of metabolomics studies, facilitating the integration of metabolomics data with other omics datasets for comprehensive molecular phenotyping.

AI-driven approaches, including machine learning and deep learning, have emerged as powerful tools for analyzing complex metabolomics data and extracting meaningful insights. Machine learning algorithms can be applied to classify

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samples, identify biomarkers, and predict metabolic phenotypes based on metabolomics data. Deep learning models enable feature learning, dimensionality reduction, and pattern recognition in high-dimensional metabolomics datasets. By leveraging AI-driven approaches, researchers can uncover hidden patterns, associations, and interactions within metabolomics data, enabling the development of personalized dietary recommendations tailored to individual health profiles.

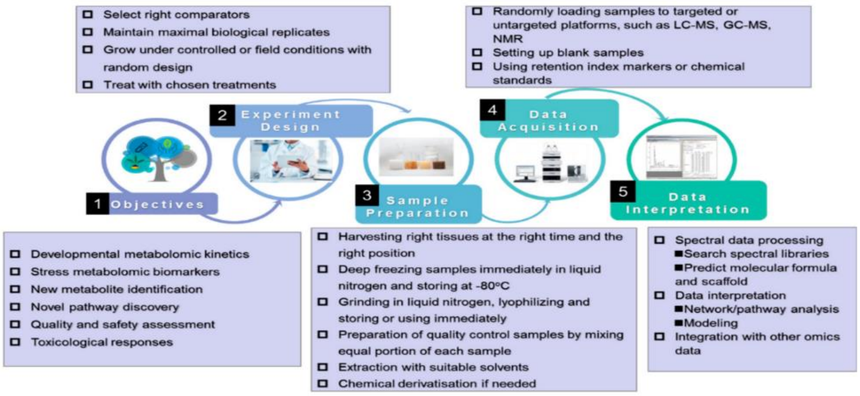

Figure 2 Steps involved for Precise Nutrition Plan.

Several studies have demonstrated the potential of AI-driven metabolomics in precision nutrition. For example, machine learning algorithms have been used to identify metabolic biomarkers associated with dietary patterns, nutrient metabolism, and disease risk. Deep learning models have been applied to predict individual responses to dietary interventions, such as low-carbohydrate diets, Mediterranean diets, and fasting regimens. By integrating metabolomics data with clinical outcomes, researchers can develop predictive models for personalized dietary recommendations that optimize health outcomes and improve patient outcomes.
Despite the promise of AI-driven metabolomics in precision nutrition, several challenges need to be addressed to realize its full potential. These include data integration, model interpretability, validation, and translation into clinical practice. Standardized data preprocessing, feature selection, and model evaluation procedures are essential for ensuring reproducibility and reliability of AI-driven metabolomics studies. Interdisciplinary collaboration between nutritionists, bioinformaticians, and data scientists is crucial for interpreting AI-driven models and translating findings into actionable dietary recommendations. Overall, the literature highlights the promise of AI-driven metabolomics in revolutionizing precision nutrition research and practice, ultimately empowering individuals to make informed dietary choices and achieve optimal health outcomes.

C.AI-Driven approaches for Analyzing Matabolomics data:- AI-driven approaches have emerged as powerful tools for analyzing metabolomics data, offering insights into complex metabolic pathways and facilitating the development of personalized dietary recommendations. Metabolomics, the systematic study of small molecules or metabolites in biological systems, provides a comprehensive snapshot of an individual's metabolic profile, reflecting the interactions between genetics, diet, lifestyle, and environmental factors. By integrating advanced analytics techniques with metabolomics data, artificial intelligence (AI) enables researchers to uncover hidden patterns, associations, and interactions within metabolomics data, ultimately contributing to the advancement of precision nutrition.
C.1 Principal Component Analysis:- One of the key AI-driven approaches for analyzing metabolomics data is Principal Component Analysis (PCA). PCA is a dimensionality reduction technique that transforms the original variables into a new set of orthogonal variables (principal components) that capture the maximum variance in the data. By reducing the dimensionality of the data while preserving the most significant information, PCA enables visualization of high-dimensional metabolomics data and identification of underlying patterns or clusters. This facilitates data exploration and interpretation, helping researchers identify biomarkers of dietary intake, nutrient metabolism, and disease risk.

Pseudocode for PCA: -
Input: Metabolomics data matrix X (m x n)

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Output: Reduced-dimensional data matrix Y (m x k)
1. Standardize the data matrix X by subtracting the mean and dividing by the standard deviation for each variable.
2. Compute the covariance matrix C = (1/m) * X^T * X.
3. Compute the eigenvectors and eigenvalues of the covariance matrix C.
4. Sort the eigenvectors in descending order based on their corresponding eigenvalues.
5. Select the top k eigenvectors corresponding to the largest eigenvalues to form the transformation matrix W.
6. Project the original data matrix X onto the k-dimensional subspace spanned by the selected eigenvectors: Y = X * W.
7. Output the reduced-dimensional data matrix Y.

C.2 Random Forest: - Another commonly used AI-driven algorithm in metabolomics analysis is Random Forest (RF). RF is an ensemble learning method that constructs a multitude of decision trees during training and outputs the mode of the classes (classification) or the mean prediction (regression) of individual trees. RF is particularly well-suited for analyzing metabolomics data due to its ability to handle high-dimensional datasets, nonlinear relationships, and interactions between variables. By leveraging the collective wisdom of multiple decision trees, RF can identify important features, classify samples, and predict metabolic phenotypes based on metabolomics data.

Pseudocode for Random Forest: -
Input: Metabolomics data matrix X (m x n), class labels y (m x 1)
Output: Predicted class labels y_pred (m x 1)
1. Initialize an empty forest F.
2. Repeat for each tree in the forest:
   a. Sample a bootstrap dataset from the original data.
   b. Randomly select a subset of features.
   c. Grow a decision tree using the bootstrap dataset and selected features.
   d. Add the tree to the forest F.
3. For each sample in the test set:
   a. Predict the class label using each tree in the forest.
   b. Aggregate the predictions to obtain the final prediction.
4. Output the predicted class labels y_pred.

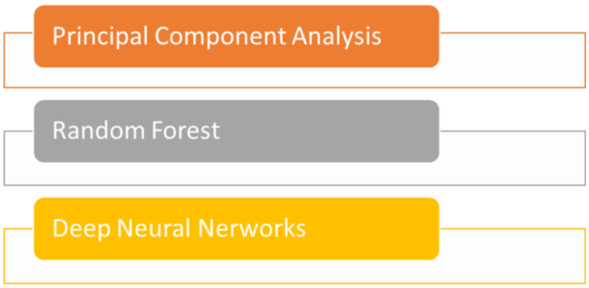

Figure 3 Approaches for AI-Driven Precision Nutrition.

C.3 Deep Neural Networks: - (DNNs) represent another class of AI-driven approaches for analyzing metabolomics data. DNNs are artificial neural networks with multiple hidden layers, capable of learning intricate patterns and representations from high-dimensional data. By processing metabolomics data through multiple layers of nonlinear transformations, DNNs can capture complex relationships between metabolites, genes, proteins, and clinical outcomes. This enables the development of predictive models for personalized dietary recommendations tailored to individual health profiles. Additionally, DNNs offer flexibility in model architecture and parameter tuning, allowing researchers to adapt the network structure to the specific characteristics of metabolomics data and research objectives.

Pseudocode for DNN: -
Input: Metabolomics data matrix X (m x n), class labels y (m x 1)

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Output: Predicted class labels y_pred (m x 1)
1. Initialize the DNN architecture with input layer, hidden layers, and output layer.
2. Randomly initialize the weights and biases of the neural network.
3. Repeat for a fixed number of iterations (epochs):
   a. Forward pass: Compute the predicted outputs (y_pred) for the input data X.
   b. Compute the loss function (e.g., cross-entropy loss) between y_pred and the true labels y.
   c. Backward pass: Compute the gradients of the loss function with respect to the network parameters.
   d. Update the weights and biases using an optimization algorithm (e.g., stochastic gradient descent).
4. Output the predicted class labels y_pred.

In addition to PCA, RF, and DNNs, other AI-driven algorithms such as support vector machines (SVM), k-nearest neighbors (KNN), and deep learning architectures like convolutional neural networks (CNN) and recurrent neural networks (RNN) are also used for metabolomics analysis. These algorithms offer diverse capabilities for data preprocessing, feature selection, classification, regression, and clustering, enabling comprehensive analysis of metabolomics data and facilitating the discovery of novel biomarkers, metabolic pathways, and therapeutic targets.

D. Challenges and Opportunities of AI-Driven Metabolomics in Precision Nutrition: -

Following are the Challenges and Opportunities of AI in Precision Nutrition: -

D.1Data Integration:

Heterogeneity: Metabolomics data often come from different platforms, such as mass spectrometry and nuclear magnetic resonance spectroscopy, each with its own data format and preprocessing steps. Integrating these diverse datasets requires harmonization and standardization to ensure compatibility and comparability across studies.

Multi-Omics Integration: Integrating metabolomics data with other omics datasets, such as genomics, proteomics, and microbiomics, poses additional challenges due to differences in data types, measurement technologies, and experimental conditions. Overcoming these challenges requires advanced computational methods for data integration and analysis.

Data Quality: Variability in sample collection, preparation, and measurement techniques can introduce noise and bias into metabolomics data. Quality control measures and rigorous data preprocessing steps are essential for ensuring the reliability and reproducibility of integrated datasets.

D.2Dimensionality:

Curse of Dimensionality: Metabolomics datasets are often high-dimensional, containing thousands of features (metabolites), which can lead to computational complexity, overfitting, and reduced interpretability. Dimensionality reduction techniques, such as PCA and feature selection methods, are used to mitigate these challenges while preserving relevant information.

Feature Selection: Identifying relevant features (metabolites) from high-dimensional data is critical for developing robust and interpretable models. Feature selection methods, such as univariate and multivariate statistical tests, as well as machine learning algorithms, help identify discriminative features associated with dietary intake, metabolic pathways, and health outcomes.

D.3Interpretability:

Black-Box Models: AI-driven models, such as deep learning architectures, often operate as black boxes, making it challenging to interpret the underlying biological mechanisms driving predictions. Interpretable machine learning techniques, such as decision trees, rule-based models, and model-agnostic interpretation methods, are needed to provide insights into feature importance, model behavior, and predictive biomarkers.

Biological Context: Integrating domain knowledge, biological pathways, and functional annotations can enhance the interpretability of AI-driven models. Incorporating prior knowledge about metabolic pathways, biochemical reactions, and physiological processes helps contextualize model predictions and identify biologically meaningful patterns.

D.4Validation:

Cross-Validation: Cross-validation techniques, such as k-fold cross-validation and leave-one-out cross-validation, are commonly used to assess the performance of AI-driven models on training data and evaluate their generalizability to unseen data. Robust validation frameworks are essential for ensuring the reliability and reproducibility of model predictions in real-world applications.

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External Validation: Independent validation cohorts and replication studies are critical for validating the predictive performance and clinical utility of AI-driven models in precision nutrition. Collaborative efforts and data sharing initiatives facilitate external validation and benchmarking of model performance across different populations and settings.

D.5Biological Variability:

Genetic Diversity: Genetic variations, such as single nucleotide polymorphisms (SNPs) and copy number variations (CNVs), contribute to inter-individual variability in metabolism and dietary response. Integrating genetic information with metabolomics data enables genotype-phenotype associations and personalized dietary recommendations based on individual genetic profiles.

Environmental Factors: Environmental factors, such as diet, lifestyle, medications, and environmental exposures, influence metabolic phenotypes and metabolic responses to dietary interventions. Accounting for environmental variability and confounding factors is essential for identifying robust biomarkers and developing personalized nutrition strategies tailored to individual health profiles.

Opportunities: -

1.Precision Nutrition: Personalized Dietary Recommendations: AI-driven metabolomics enables the development of personalized dietary recommendations tailored to individual metabolic profiles, genetic backgrounds, and health goals. By integrating metabolomics data with clinical outcomes and lifestyle factors, researchers can identify optimal dietary interventions for improving health outcomes and preventing diet-related diseases.

2.Biomarker Discovery: Early Detection and Risk Stratification: AI-driven metabolomics facilitates the discovery of novel metabolic biomarkers associated with dietary intake, nutrient metabolism, and disease risk. Biomarker discovery enables early detection, risk stratification, and targeted interventions for metabolic disorders, such as obesity, diabetes, cardiovascular disease, and cancer.

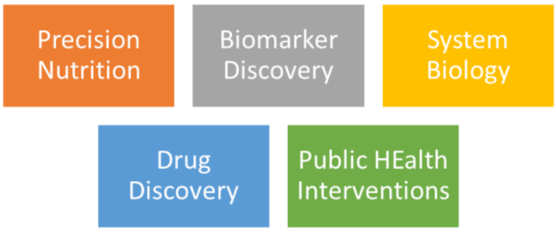

Figure 4 Opportunities for AI-Driven Precision Nutrition.

3.Systems Biology:. Metabolic Network Analysis**:** AI-driven metabolomics enables systems-level analysis of metabolic networks, pathways, and interactions. By integrating multi-omics data and biological knowledge databases, researchers can unravel the complexity of metabolic regulation, identify key nodes for therapeutic targeting, and develop precision medicine approaches for metabolic diseases.

4.Drug Discovery: Pharmacometabolomics: Metabolomics-based drug discovery leverages AI-driven approaches to identify and characterize bioactive compounds in foods, supplements, and pharmaceuticals. Targeted nutritional interventions and pharmacological interventions can modulate metabolic pathways, improve treatment outcomes, and optimize drug efficacy and safety profiles for metabolic disorders and chronic diseases.

5.Public Health Interventions: Population-Level Impact: AI-driven metabolomics has implications for public health interventions, including dietary guidelines, food policy, and nutritional education programs. Tailoring dietary recommendations based on individual metabolic profiles and genetic backgrounds can promote healthier eating habits, prevent diet-related diseases, and reduce the burden of metabolic disorders on a population scale.

E. Future Directions and Emerging Trends: Looking ahead, several emerging trends and future directions are shaping the field of AI-driven metabolomics for precision nutrition. These include the integration of multi-omics data, the development of explainable AI models, the adoption of cloud-based platforms, and the democratization of data science tools. Integrating metabolomics data with other omics datasets, such as genomics, proteomics, and microbiomics, holds promise for uncovering complex interactions between genes, environment, and lifestyle factors in shaping metabolic phenotypes. Moreover, developing explainable AI models that provide interpretable results and actionable insights is crucial for translating AI-driven findings into clinical practice and public health interventions. Cloud-based platforms and data science tools, such as open-access databases, collaborative platforms, and reproducible workflows, facilitate data sharing, collaboration, and knowledge dissemination in the field of precision nutrition. By embracing these trends and leveraging AI-driven approaches, researchers can accelerate the pace of discovery, innovation, and translation in precision nutrition, ultimately empowering individuals to make informed dietary choices and achieve optimal health outcomes.

Conclusion: - In conclusion, AI-driven metabolomics represents a groundbreaking approach to precision nutrition, offering the potential to revolutionize the way we understand, personalize, and optimize dietary recommendations based on individual health profiles. Through the integration of advanced analytics techniques with metabolomics data, researchers can uncover intricate relationships between dietary intake, metabolic pathways, and health outcomes, paving the way for tailored dietary interventions that optimize health and well-being. The challenges of data integration, dimensionality, interpretability, validation, and biological variability in AI-driven metabolomics present formidable obstacles, but they also provide opportunities for innovation and advancement. By addressing these challenges through interdisciplinary collaboration, methodological advancements, and rigorous validation frameworks, researchers can harness the full potential of AI-driven metabolomics to develop robust predictive models and actionable insights for precision nutrition. Despite the complexity of human metabolism and the diversity of individual health profiles, AI-driven metabolomics offers exciting opportunities for personalized dietary recommendations that account for genetic, environmental, and lifestyle factors. By leveraging metabolomics data in conjunction with other omics datasets, such as genomics, proteomics, and microbiomics, researchers can gain deeper insights into the interplay between genetics, metabolism, and dietary response, enabling the development of targeted interventions for metabolic disorders and chronic diseases. Biomarker discovery, systems biology analysis, drug discovery, and public health interventions are among the key areas of opportunity for AI-driven metabolomics in precision nutrition. By identifying novel metabolic biomarkers, unraveling metabolic networks, characterizing bioactive compounds, and informing public health policies, AI-driven metabolomics has the potential to improve health outcomes, reduce healthcare costs, and enhance quality of life for individuals and populations worldwide. In summary, AI-driven metabolomics holds tremendous promise for advancing precision nutrition research and practice, empowering individuals to make informed dietary choices based on their unique metabolic profiles and health goals. By embracing the challenges and opportunities presented by AI-driven metabolomics, we can unlock new insights into human metabolism, enhance the effectiveness of dietary interventions, and ultimately promote optimal health and well-being for all.

Reference: -

[1] Wishart, D.S., Feunang, Y.D., Marcu, A. et al. HMDB 4.0: the human metabolome database for 2018. Nucleic Acids Res 46, D608–D617 (2018). doi:10.1093/nar/gkx1089.

[2] Zhang, A., Sun, H., Wang, X. Serum metabolomics as a novel diagnostic approach for disease: a systematic review. Anal Bioanal Chem 404, 1239–1245 (2012). doi:10.1007/s00216-012-6206-z.

[3] Johnson, C.H., Ivanisevic, J., Siuzdak, G. Metabolomics: beyond biomarkers and towards mechanisms. Nat Rev Mol Cell Biol 17, 451–459 (2016). doi:10.1038/nrm.2016.25.

[4] Wishart, D.S. Emerging applications of metabolomics in drug discovery and precision medicine. Nat Rev Drug Discov 15, 473–484 (2016). doi:10.1038/nrd.2016.32.

[5] Nicholson, J.K., Holmes, E., Kinross, J., et al. Host-gut microbiota metabolic interactions. Science 336, 1262–1267 (2012). doi:10.1126/science.1223813.

[6] Mardinoglu, A., Boren, J., Smith, U. Confounding effects of metformin on the human gut microbiome in type 2 diabetes. Cell Metab 23, 10–12 (2016). doi:10.1016/j.cmet.2015.10.014.

[7] Kanehisa, M., Goto, S. KEGG: Kyoto Encyclopedia of Genes and Genomes. Nucleic Acids Res 28, 27–30 (2000). doi:10.1093/nar/28.1.27.

[8] Uhlen, M., Fagerberg, L., Hallstrom, B.M., et al. Proteomics. Tissue-based map of the human proteome. Science 347, 1260419 (2015). doi:10.1126/science.126041.

[9] Chong, J., Soufan, O., Li, C., et al. MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. Nucleic Acids Res 46, W486–W494 (2018). doi:10.1093/nar/gky310

[10] Sun, H., Wang, M., Zhang, A., et al. UPLC-Q-TOF-HDMS analysis of constituents in the root of two kinds of Aconitum using a metabolomics approach. Phytochem Anal 21, 392–402 (2010). doi:10.1002/pca.1207.
[11] Wishart, D.S., Tzur, D., Knox, C., et al. HMDB: the Human Metabolome Database. Nucleic Acids Res 35, D521–D526 (2007). doi:10.1093/nar/gkl923.
[12] Wishart, D.S., Jewison, T., Guo, A.C., et al. HMDB 3.0—The Human Metabolome Database in 2013. Nucleic Acids Res 41, D801–D807 (2013). doi:10.1093/nar/gks1065.
[13] Smith, C.A., O'Maille, G., Want, E.J., et al. METLIN: a metabolite mass spectral database. Ther Drug Monit 27, 747–751 (2005). doi:10.1097/01.ftd.0000179845.53213.39.
[14] Horai, H., Arita, M., Kanaya, S., et al. MassBank: a public repository for sharing mass spectral data for life sciences. J Mass Spectrom 45, 703–714 (2010). doi:10.1002/jms.1777.
[15] Smith, C.A., Maille, G.O., Want, E.J., et al. METLIN: a metabolite mass spectral database. Ther Drug Monit 27, 747–751 (2005). doi:10.1097/01.ftd.0000179845.53213.39.
[16] .Kanehisa, M., Goto, S., Furumichi, M., et al. KEGG for representation and analysis of molecular networks involving diseases and drugs. Nucleic Acids Res 38, D355–D360 (2010). doi:10.1093/nar/gkp896
[17] Wishart, D.S., Knox, C., Guo, A.C., et al. DrugBank: a comprehensive resource for in silico drug discovery and exploration. Nucleic Acids Res 34, D668–D672 (2006). doi:10.1093/nar/gkj067
[18] Wishart, D.S., Knox, C., Guo, A.C., et al. HMDB: a knowledgebase for the human metabolome. Nucleic Acids Res 37, D603–D610 (2009). doi:10.1093/nar/gkn810
[19] Wishart, D.S., Jewison, T., Guo, A.C., et al. HMDB 3.0—The Human Metabolome Database in 2013. Nucleic Acids Res 41, D801–D807 (2013). doi:10.1093/nar/gks1065
[20] Wishart, D.S., Feunang, Y.D., Marcu, A. et al. HMDB 4.0: the human metabolome database for 2018. Nucleic Acids Res 46, D608–D617 (2018). doi:10.1093/nar/gkx1089