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Authors

Gan, Junai

Siegel, Justin B

German, J Bruce

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Molecular annotation of food – towards personalized diet and precision health

Junai Gan^a, Justin B. Siegel^{b,c,d}, J. Bruce German^{a,e,*}

^aDepartment of Food Science and Technology, University of California, Davis, CA, United States

^bDepartment of Chemistry, University of California, Davis, CA, United States

^cDepartment of Biochemistry and Molecular Medicine, University of California, Davis, CA, United States

^dGenome Center, University of California, Davis, CA, United States

^eFoods for Health Institute, University of California, Davis, CA, United States

Abstract

Background—Personalized diet requires matching human genotypic and phenotypic features to foods that increase the chance of achieving a desired physiological health outcome. New insights and technologies will help to decipher the intricacies of diet-health relationships and create opportunities for breakthroughs in dietary interventions for personal health management.

Scope and Approach—This article describes the scientific progress towards personalized diet and points out the need for integrating high-quality data on food. A framework for molecular annotation of food is presented, focusing on what aspects should be measured and how these measures relate to health. Strategies of applying trending technologies to improve personalized diet and health are discussed, highlighting challenges and opportunities for transforming data into insights and actions.

Key Findings and Conclusions—The goal of personalized diet is to enable individuals and caregivers to make informed dietary decisions for targeted health management. Achieving this goal requires a better understanding of how molecular properties of food influence individual eating behavior and health outcomes. Annotating food at a molecular level encompasses characterizing its chemical composition and modifications, physicochemical structure, and biological properties. Features of molecular properties in the food annotation framework are applicable to varied conditions and processes from raw materials to meals. Applications of trending technologies, such as omics techniques, wearable biosensors, and artificial intelligence, will support data collection, data analytics, and personalized dietary actions for targeted health management.

Keywords

Diet; Food; Personalized nutrition; Health; Molecular property; Data

*Corresponding author at: Foods for Health Institute, Department of Food Science and Technology, University of California, Davis, CA 95616, USA. jbgerman@ucdavis.edu.

Introduction

In the past two decades, the success of human genome project and the initiative on precision medicine have accelerated progress towards personalized healthcare (Francis S. Collins, Green, Guttmacher, & Guyer, 2003; F. S. Collins & Varmus, 2015). Applications of omics technologies such as genomics, epigenomics, transcriptomics, proteomics, and metabolomics in health research have not only advanced the field of medicine, but also revolutionized nutritional sciences (German, Zivkovic, Dallas, & Smilowitz, 2011; Kellogg, Dunn, & Snyder, 2018). Capturing genotypic and phenotypic characteristics of individuals has improved our understanding of the diverse effects of nutrition on health, which raised the excitement for personalized diet to address individual variations. Although the importance of diet on health has attracted increasing attention, the complexity and variability of this relationship has not been fully recognized. Diet and food are complex systems that are more than the sum of nutritional components. Food properties can directly influence individual dietary intake, affect molecular behaviors along the gastrointestinal tract, stimulate various metabolic and physiological responses, and ultimately have an impact on one's health and overall quality of life in both short and long term. Characterizing diet and food at the molecular level is equally important as capturing individual variations in response to consuming them. Integrating the information of both input and output is necessary to decipher the impact of diet on health. Such knowledge will transform the potential of personalized diet for precision health management.

This article describes the scientific progress towards personalized diet and points out the need for integrating high-quality and well-annotated data on food. A framework for molecular annotation of food is presented, proposing key measurements of food based on implications for diet and health. Strategies of applying trending technologies to improve the predictive power of personalized diet for precision health are discussed, highlighting challenges and opportunities for transforming data into insights and actions.

Trajectory towards personalized diet

In the most basic sense, personalized diet requires matching human genotypes and phenotypes to a diet that will increase the chance of achieving desired physiological outcomes. As we move towards this goal, two aspects are important: one – the ability to accurately measure the genetic and molecular features of a human; and two – the ability to accurately measure molecular properties of food and diet (Fig. 1).

On the first front, measuring the genetic and molecular features of a human, the ability to sequence the human genome at the beginning of the 21st century started providing new insights into the molecular basis of diet-related diseases, revolutionizing nutrition research. There has been growing awareness of interactions between nutrients and genes. Accordingly, nutrigenetics and nutrigenomics have arisen as scientific fields to explore the nutrient-gene interactions that cannot be addressed by classical epidemiological and physiological approaches (Muller & Kersten, 2003; Mutch, Wahli, & Williamson, 2005). Advances by these fields and evidence of nutrient-gene interactions have been recently reviewed (Vyas, Singh, Singh, Kumar, & Dhaliwal, 2018). With public databases, data mining and integrative

analysis of gene expression profiles in response to food have assisted in identifying molecular mechanisms of nutrigenomics studies and designing dietary recommendations (Martin-Hernandez, Reglero, & Davalos, 2018; Zheng, Ni, Li, Chow, & Panagiotou, 2017). In addition to mapping the human blueprint, molecular measurement of human phenotypes with omics technologies has been providing detailed information on the transcriptome, proteome, metabolome, and microbiome of individuals (Karczewski & Snyder, 2018). Capturing genotypic and phenotypic characteristics of individuals has improved our understanding of the diverse effects of nutrition on health, which raised enthusiasm for personalized diet to address individual variations. For instance, postprandial glycemic responses have been successfully predicted based on personal blood parameters, dietary habits, anthropometrics, physical activity, and gut microbiome, providing opportunities for dietary interventions to control postprandial blood glucose and its metabolic consequences (Zeevi, et al., 2015).

On the second front, measuring the molecular properties of food, less progress has been made. Currently, dietary assessment methods based on self-reported data are still the standard in the field; such dietary assessments do not provide accurate molecular information and have large measurement error (Subar, et al., 2015). Inaccurate dietary data are a major impediment to research on diet and health. However, this is going to be changed. As significant advances of omics technologies driven by the healthcare industry, the cost of a full omics analysis of complex matrices is becoming affordable. These technologies will be increasingly utilized to evaluate food and provide an unprecedented insight into the molecular properties of our diet and the physiological outcomes observed for a specific individual. The next section of this article focuses on the molecular properties of food that need annotation (Fig. 2) and their relevance to diet and health (Table 1).

Once full molecular annotations of human and diet have begun, the key will rely on how to utilize these datasets. Currently, the focus on personalized nutrition is to provide dietary recommendations based on one's nutritional needs with an implicit assumption that food is simply a mixture of nutritional ingredients. There is a growing realization that diet is more than the sum of its parts. For instance, differences in food structures of the same ingredients affect digestion kinetics, absorption dynamics, metabolic and physiological responses (Augustin, et al., 2015; Bourlieu, et al., 2015; Fardet, Dupont, Rioux, & Turgeon, 2018; Parada & Aguilera, 2007). In addition, food structures affect personal perception and preference (Kaufmann & Palzer, 2013). Therefore, food research needs to shift from an ingredient-centric model to an integrated approach considering the entire diet. Annotating the chemical components and modifications, physical structures, and biological properties of food will lead to a diversity of dietary options to meet nutritional needs along with individual, social, and cultural preferences. High-quality and well-annotated data on food will be instrumental in developing personalized diet that is effective in behavioral change to benefit health.

Framework for food annotation – what to measure and why it matters

Food composition

Food composition focuses on the amounts of chemical components in food. Many countries and regions have food composition databases distributed by government agencies, such as the United States Department of Agriculture (USDA) Food Composition Databases (Haytowitz & Pehrsson, 2018). The values for food composition data are typically chosen by essentiality and determined by standard chemical analyses (Elmadfa & Meyer, 2010). Although food composition data are often only available for energy, major nutritional categories, and some important nutrients, these data have been providing foundations for health professionals, nutrition educators, policy makers, agricultural producers, food manufacturers, and consumers for decision making (Charrondiere, et al., 2016; Elmadfa & Meyer, 2010). Food composition databases need continuous maintenance and development to keep pace with scientific discoveries on dietary components, eating habits of the growing population, and food products in the changing marketplace (Charrondiere, et al., 2016; Elmadfa & Meyer, 2010; Haytowitz & Pehrsson, 2018). Towards precision health management, more detailed characterization of chemical components of food is needed. For example, not only the total amount but also specific types of proteins matter to infant health. Infant formulas have been improved from only matching the total protein content to better matching the protein profile of human milk, such as altering the whey-to-casein ratio of cow milk proteins and adjusting the proportion of specific whey proteins like α -lactalbumin in formulas (Lien, 2003). Clinical data showed that enriching with α -lactalbumin improves the protein quality of the formula and better supports age-appropriate growth of the infant (Trabulsi, et al., 2011). In terms of carbohydrate composition, human milk contains a complex mix of oligosaccharides that favor specific *Bifidobacterium* species in the infant gut, while formulas with the addition of simple galacto- and fructo-oligosaccharides do not mimic the breastfed-like infant gut microbiome, showing that specific dietary components alter gene-encoded functions of the developing gut microbiome (Baumann-Dudenhoeffer, D'Souza, Tarr, Warner, & Dantas, 2018). Annotating chemical components of food more precisely and holistically will be essential to decipher diet-health relationships.

Chemical modifications

Characterizing chemical modifications of molecules requires analytical approaches such as mass spectrometry, infrared spectroscopy, and nuclear magnetic resonance spectroscopy that are more precise than compositional measurements. Chemical modifications and interactions of food molecules affect sensory and nutritional properties of the diet. For example, phosphorylation and glycosylation of food proteins alters their solubility, heat stability, foaming ability, emulsifying activity, digestibility, and immunogenicity (Gan, Bornhorst, Henrick, & German, 2018; Li, Enomoto, Hayashi, Zhao, & Aoki, 2010). Maillard reaction between amino acids and reducing sugars is common in food processing. Maillard reaction products contribute to colors and flavors in food, and they can be either beneficial or toxic as shown in pre-clinical and clinical studies; their characterization, occurrence, and health effects are under ongoing investigation (Tamanna & Mahmood, 2015; Tessier & Birlouez-Aragon, 2012). Phosphorylation, glycosylation, oxidation, disulfide crosslink, and other chemical bonding are common modifications of dietary molecules. Dynamic changes of

these molecular modifications occur during food production, processing, storage, preparation, and digestion. In turn, chemical modifications shape the sensory and functional attributes of the food, influence personal preferences and consumption behavior, and ultimately affect individual health outcomes.

Food structure

Food structure or food microstructure describes the spatial arrangement of food constituents and their interactions. The architecture of molecules in food determines its form, such as foam, gel, emulsion, suspension, solution, and solid. Studies on food structures often utilize microscopic techniques to visualize the geometric organization of molecules and rheological techniques to investigate the molecular interactions. Different crystal packing configurations of cocoa butter lead to a superb chocolate with desired gloss or a bloomed chocolate with an unappealing whitish haze (Delbaere, Van de Walle, Depypere, Gellynck, & Dewettinck, 2016). Differences in emulsion structures of fat droplets in maternal milk and infant formulas modify the kinetics of lipid and protein digestion (Bourlieu, et al., 2015). Food matrix impacts carbohydrate metabolism, resulting in varied post-prandial blood glucose response; glycemic index, the concept that connects food structure and physiological response, has clinical successes and profound implications for dietary interventions and health management (Augustin, et al., 2015; Zeevi, et al., 2015). Annotating structural transformations of food from raw material to processing and digestion will empower food structure engineering to design diet with specific nutritional, physical, and sensory attributes addressing tailored needs (Kaufmann & Palzer, 2013). Sous vide cooking, the method of preparing food in vacuumized pouches using precisely controlled heating, is a success in controlling food safety, texture, taste, and nutrition based on the understanding of structural changes of food as a function of temperature and time (Baldwin, 2012).

Biological properties

Biological properties of food refer to beneficial or adverse effects extending beyond its nutritional value. A considerable diversity of biological activities has been discovered from numerous dietary components. Proteins in human milk, for instance, exert various beneficial bioactivities, such as enzyme activities, growth stimulation, immune modulation, and antimicrobial activities (Lonnerdal, 2013). Breastfed infants receive bioactive enzymes from their diet and these enzymes are likely to function in their gastrointestinal tract (Dallas, Murray, & Gan, 2015). Worth noting is that pasteurization and freeze-thaw cycles of donor human milk damage the composition of proteins, their activities and potentially their functions (Ballard & Morrow, 2013). Besides beneficial biological properties, food proteins also associate with adverse effects. For example, dietary glutes induce celiac diseases in genetically predisposed persons (Shan, et al., 2002), and food allergens cause severe allergic reactions in susceptible populations (Sicherer & Sampson, 2014). In addition, food contains microbes which can be valuable as starters for fermentation and as probiotics for consumers; microbes in food can also be undesirable for causing food spoilage and causing foodborne illnesses (Ray & Bhunia, 2013). Therefore, annotating both beneficial and adverse biological properties of food from raw materials to final products will support diet and health management.

Applications of trending technologies – challenges and opportunities

Collecting data from various sources

Diet and health are multifactorial dynamic systems in an interconnected network. Capturing the variations of their key features as well as the associated factors is necessary to obtain a holistic overview for diet and health management. Although this task is challenging to complete, exploiting advanced technologies for data collection will provide a more comprehensive view of diet and health. Discussion in this section focuses on data collection for food and diet (Fig. 3).

Food analysis in the 21st century has been revolutionized by the development of sophisticated analytical instrumentation, the advancement of high-throughput sequencing techniques, and their applications in food science (Ercolini, 2013; Garcia-Canas, Simo, Herrero, Ibanez, & Cifuentes, 2012). Together with classical methodologies, these diverse technologies empower researchers to annotate chemical, physical, and biological properties of food with increased precision, accuracy, sensitivity, and specificity. Since each technology alone cannot capture the entire intricacy of food and diet, integration of multiple technologies has emerged in food research. This integrative approach introduces new challenges particularly in data management; thus, new informatics infrastructures are needed to facilitate its implementation.

Portable electronic devices enable individuals to collect dietary data anywhere and anytime. Taking pictures to keep track of food intake or entering consumption data in a timely manner will improve the accuracy of dietary assessment. Improvements on portable food analyzers like near-infrared spectrometers (dos Santos, Lopo, Páscoa, & Lopes, 2013) are useful for estimating diet composition in place. Furthermore, large technology companies are expanding investment in wearable biosensing devices. Despite concerns for their reliability and effectiveness, wearable biosensors offer enormous potential for physiological monitoring (Ajami & Teimouri, 2015; Patel, Asch, & Volpp, 2015). One application of wearable biosensors is to monitor individual dietary intake and its impact on physiological responses.

Gaining insights through data analytics

A challenge in the era of big data is to gain meaningful insights through data analytics. Data on food and diet can be generated from near-infrared spectroscopy, mass spectrometry, transmission electron microscopy, texture analyzers, DNA sequencers, cell cultures, bioactivity assay kits, smart phones and mobile apps, and wearable devices and sensors, etc. Because of the large volume and diverse data types, analyzing such food and diet data is overwhelming. The conceptual framework of big data analytics is applicable. In short, raw data across disparate data sources are transformed, input to analytics platforms, and finally applied to guiding decisions (Raghupathi & Raghupathi, 2014).

The explosive growth of machine learning algorithms and artificial intelligence techniques is renovating the applications of medical data (Esteva, et al., 2019; He, et al., 2019). Adapting concepts and techniques developed in medicine will accelerate innovations in food and diet. For example, convolutional neural network, an algorithm used to process medical images

(Gurovich, et al., 2019; Kermany, et al., 2018), can be employed to analyze food pictures; natural language processing, a computational method for processing text from electronic medical records (Liao, et al., 2015), is suitable for processing electronic dietary records.

Interpretation and prediction based on the analysis is critical for transforming information into actionable insights that individuals can use to guide their dietary decisions. Statistical models specifically for data on food properties and dietary patterns need to be developed and validated. A further step for more personalized and precise dietary predictions relies on the integration of food data with personal health data. The convergence of all these data poses computational, statistical, ethical, and regulatory challenges; finding practical solutions for these challenges will create opportunities for precision health management.

Supporting actions upon personalized insights

It is difficult to effectively change behavior that is sustained towards improved health (Celis-Morales, Lara, & Mathers, 2015; Patel, et al., 2015). A gap exists between providing personalized dietary advice and altering individual eating behavior. To bridge this gap, technology-based strategies are proposed for effective use of personalized dietary insights to facilitate healthy eating behavior.

Increasing evidence suggests that incorporating behavior change techniques into dietary interventions facilitates food behavior change (Celis-Morales, et al., 2015; Spahn, et al., 2010). Information and communication technology may boost the efficiency of the behavior change techniques. For example, goal setting and reward strategies can be embedded in software programs that allow customization based on personal health expectations and food preferences. Monitoring and feedback are achieved by wearable biosensing devices, like a biosensor that monitors blood glucose levels and eating activities and that alerts the user when blood glucose level is out of the normal range. Social support can be attained by a social network that encourages individuals to share meal plans and images with others. In addition, personalized diet education can be delivered through web-based interactive learning sites.

Besides individual factors, food environments contribute to eating behavior (Story, Kaphingst, Robinson-O'Brien, & Glanz, 2008). Incorporating personalized diet into the local food system will support individuals to follow the healthy dietary advice. If the delivery system of local grocery stores is connected to the personalized dietary planning, and if all restaurants can provide meals that are prepared based on the personalized advice, then a personalized dietary plan is more likely to be on one's plate.

Conclusions

Diet is more than the sum of its parts, and food is not merely a mixture of nutritional components. Instead, the chemical, physical, and biological characteristics of food endow it with sensory, safety, and functional attributes that extend beyond nutritional value. Foods with similar ingredients but dissimilar structures, such as pre-cooked vs. cooked rice with distinct starch structures and raw vs. homogenized milk with different fat globule sizes, differ in digestion kinetics, absorption dynamics, metabolic and physiological responses

(Augustin, et al., 2015; Fardet, 2015; Fardet, et al., 2018). Food preference varies from person to person, and this should be considered as an important dimension for personalized diet. We argue that the goal of personalized diet is enabling individuals and caregivers to make informed dietary decisions for targeted health management. Achieving this goal requires a better understanding of how molecular properties of food affect individual eating behavior and health outcomes. Annotating food at a molecular level encompasses characterizing its chemical composition and modifications, physicochemical structures, and biological properties. Molecular properties of food change dynamically during food production, processing, storage, preparation, digestion, and absorption. Features of molecular properties in the food annotation framework are applicable to varied conditions and processes from raw materials to meals. Constructing and updating databases for food requires continuous and collaborative efforts. Comprehensive molecular annotation of food is creating a map that will empower researchers to identify diet-health relationships, engineers to design diet for tailored needs, and individuals to make personalized dietary decisions for health management.

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Highlights

- Scientific and technological advances accelerate progress towards precision health.
- Nutrigenetics and nutrigenomics capture individual variations.
- The complexity of diet and food is not fully recognized.
- A framework for annotating molecular properties of food is presented.
- Trending technologies can be applied to personalized diet and health management.

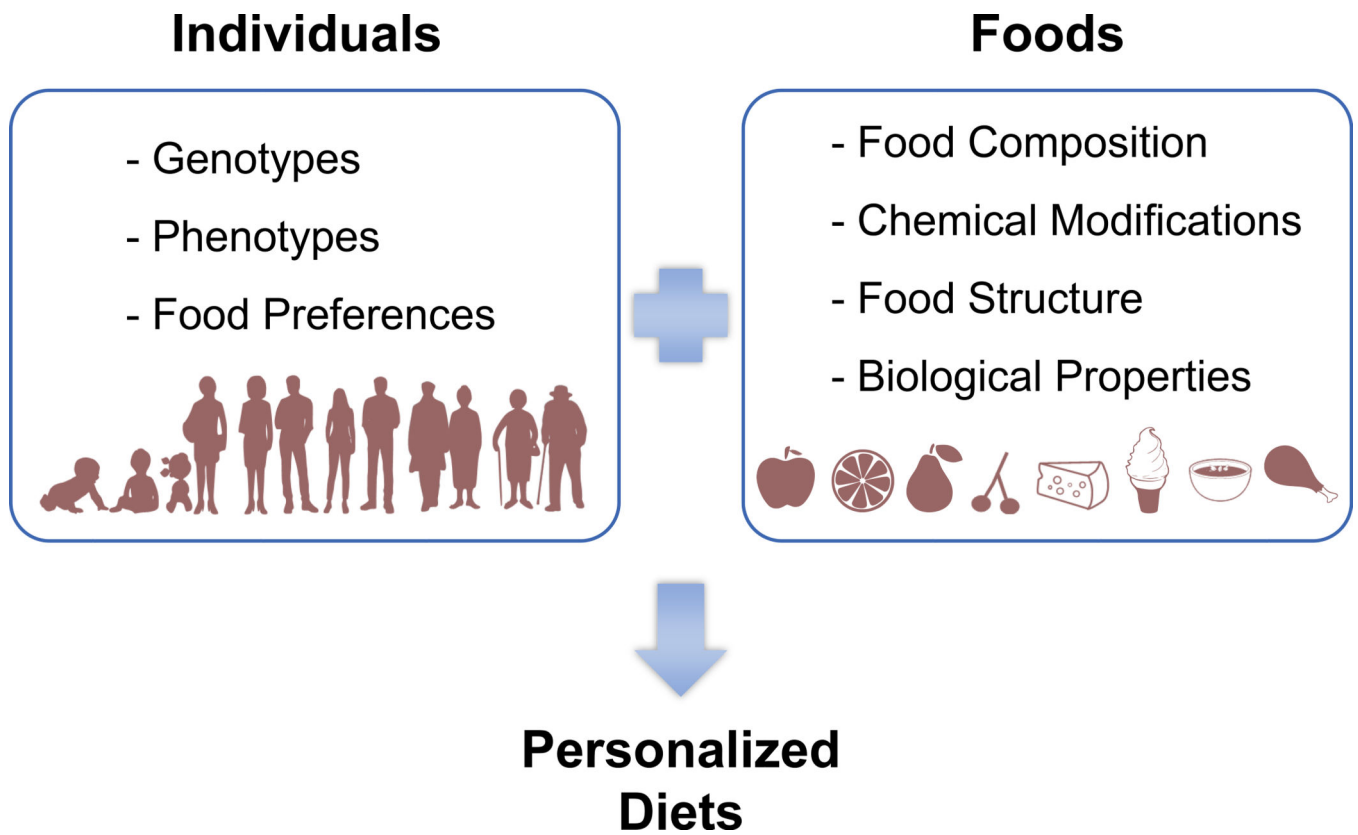


Fig. 1.
Key aspects for personalized diets.

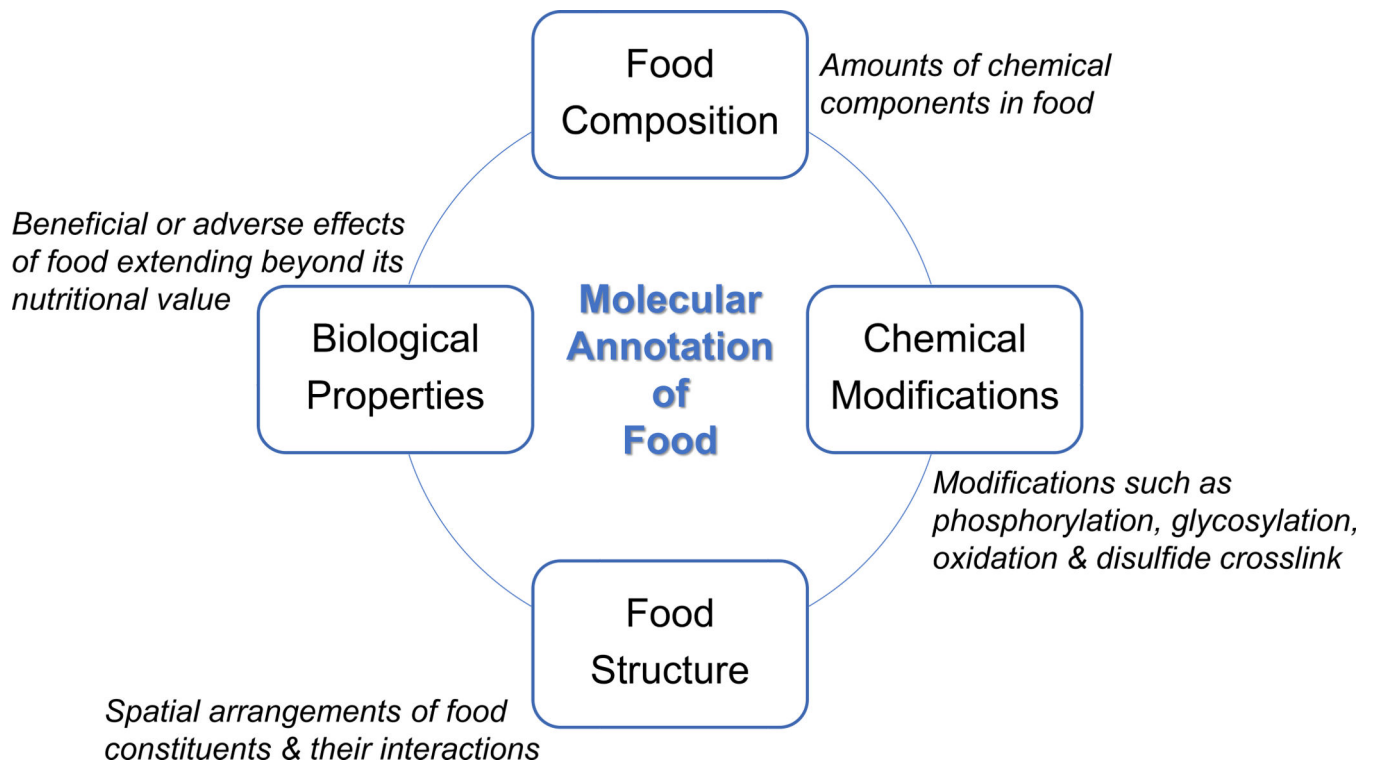


Fig. 2.
Framework for annotating molecular properties of food.

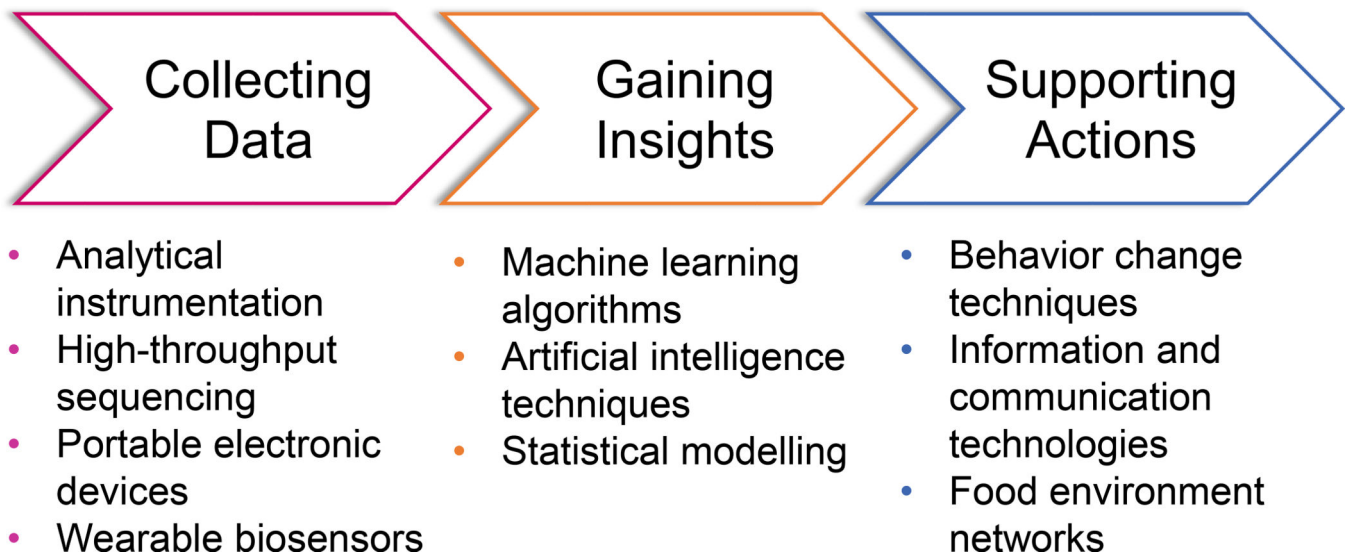


Fig. 3.
Applying trending technologies in utilizing information of food for health management.

Table 1.

Molecular properties of food and their health relevance.

Molecular properties	Examples of health relevance	References
Food composition	Food composition databases provide foundations for dietary guidelines.	(Charrondiere, et al., 2016; Elmadfa & Meyer, 2010)
	Infant formulas enriched with α -lactalbumin better match the protein profile of human milk and support age-appropriate growth of infants.	(Trabulsi, et al., 2011)
	Compared to human milk with a complex mix of oligosaccharides, formulas with simple galacto- and fructo-oligosaccharides predict distinct gene-encoded functions of the infant gut microbiome.	(Baumann-Dudenhoeffer, D'Souza, Tarr, Warner, & Dantas, 2018)
Chemical modifications	Phosphorylation and glycosylation of food proteins alter digestibility and immunogenicity.	(Gan, Bornhorst, Henrick, & German, 2018; Li, Enomoto, Hayashi, Zhao, & Aoki, 2010)
	Diverse maillard reaction products exhibit antioxidative, bactericidal and carcinogenic effects.	(Tamanna & Mahmood, 2015; Tessier & Birlouez-Aragon, 2012)
Food structure	Different crystal packing configurations of cocoa butter change sensory perceptions and preferences.	(Delbaere, Van de Walle, Depypere, Gellynck, & Dewettinck, 2016)
	Differences in emulsion structures of fat droplets modify the kinetics of lipid and protein digestion.	(Bourlieu, et al., 2015)
	Food matrix impacts carbohydrate metabolism, resulting in varied post-prandial blood glucose response.	(Augustin, et al., 2015; Zeevi, et al., 2015)
Biological properties	Human milk proteins exert various bioactivities including enzyme activities, growth stimulation, immune modulation, and antimicrobial activities.	(Lonnerdal, 2013)
	Dietary glutes induce celiac diseases in genetically predisposed persons.	(Shan, et al., 2002)
	Some microbes in foods are probiotics while other microbes can cause foodborne illnesses.	(Ray & Bhunia, 2013)