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4 5 Foodomics: Advances in product testing in agri-food supply chains

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6 Summary

7 This chapter is written to describe the concept of product testing in agri-food supply chains 8 and the methods that are being developed to identify instances of product non-conformance 9 with either regulatory requirements, market requirements or both. The emergence of a range of 10 new technologies provides opportunity to build on existing product testing protocols and offer 11 complementary alternative and rapid testing of food which can provide assurance that food 12 products are consistently what they are purported to be. Microbiological contamination will 13 not be considered in this chapter. Effective and targeted product testing also acts as a potential 14 deterrent against food safety incidents and food fraud. The chapter also introduces the term 15 "foodomics" and what this means in terms of smart agri-food supply chains.

16 **1. Introduction**

17 Defining product characteristics and then undertaking product testing to confirm that the 18 food product is within an agreed specification or meets a specific standard is of value if the 19 results obtained can be associated with a given batch or lot of food (Zwietering et al. 2016). 20 ISO 9001:2015 Quality Management Systems: fundamentals and vocabulary defines quality 21 as the degree to which a set of inherent [innate] characteristics of an object [in this case food] 22 fulfils requirements i.e. conforms with a given specification or set of criteria. Assessment of 23 conformity can be via inspection (assessment of characteristics and whether they conform to 24 specified requirements); *monitoring* (determining the status of the product i.e. is it compliant or non-compliant) and verification (confirmation that objective evidence is available to 25 26 demonstrate that a product meets specified requirements). Determination of the status of a 27 product can be via on-line, off-line or retrospective assessment. This can include product 28 testing (inspection), visual inspection or assessment of evidence such as certificates of analysis 29 that vouch for the conformity of the product (verification). In many food supply chains that 30 follow an assurance approach, verification activities of processes and documentation have 31 replaced product inspection activities. One of the reasons for this is that product testing can be 32 costly and introduce time delays in food supply chains that are highly cost sensitive. These 33 food chains focus on a "just in time" approach to minimise stock holding of perishable or short 34 shelf-life products from a food safety and quality viewpoint, and excessive stockholding of 35 long-life products to mobilise financial resources (Manning and Soon, 2014).

36 The design and implementation of preventative assurance approaches to address food 37 safety and quality has provided a high degree of confidence in the food safety and quality 38 management systems employed and replaced reactive, control-based final product testing 39 (Manning et al. 2019). This preventative assurance approach has also utilised third party certification (TPC) audits to assess organisational compliance with recognised normative 40 41 system standards. For a wider explanation of the terms used in this chapter see Table 1. The Elliott Review, following the 2013 Horsemeat Scandal, concluded that the quality and 42 43 completeness of TPC audits was variable and that these audits alone would not deliver effective 44 verification of integrity in the food supply chain unless they were combined with other 45 activities such as product testing (Elliott Review 2014; Manning and Monaghan, 2019). 46 Food integrity has been variously described as whether the food product is exactly what is 47 stated on the label (Ali & Suleiman, 2018) or simply what it purports to be (Manning, 2016). 48 Manning (2016) defines food integrity as having four components product integrity, process 49 integrity, data integrity and people integrity. Some of these components are considered in this chapter and other chapters in the book. Food integrity is also considered to be: 50

51 "a general term for sound, nutritive, healthy, tasty, safe, authentic, traceable, as well as

- 52 ethically, safely, environment-friendly, and sustainably produced foods (Rychlik et al., 2018,
- 53

p. 49).

54 Table 1. Glossary of terms associated with quality, quality control and quality assurance

- 55 (Source: <u>https://www.iso.org/obp/ui</u>,)
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Term	Definition
Characteristics	Distinguishing feature which can be inherent or assigned, quantitative or qualitative.
	Characteristics can be physical (chemical, biological); sensory (organoleptic); behavioural
	(integrity, honesty); temporal (reliability); or functional (preservative, flavour, colour etc.)
Conformity	Fulfilment of a requirement
Data	Facts about an object
Defect	Nonconformity related to an intended or specified use
Determination	Activity to find out one or more characteristics and their characteristic values
Document	Information and the medium on which it is contained
Information	Meaningful data
Inspection	Determination of conformity to specified requirements
Monitoring	Determining the status of a system, a process, a product, a service or an activity
Nonconformity	Non-fulfilment of requirement
Object	Can be material e.g. food ingredient, product, service or perceived e.g. status.
Objective	Data supporting the existence or veracity of something
evidence	
Quality	Degree to which a set of inherent characteristics of an object fulfils requirements
	an object (3.6.1) fulfils requirements (3.6.4)
Quality	Part of quality management focused on providing confidence that quality requirements
assurance	will be fulfilled.
Quality control	Part of quality management focused on fulfilling quality requirements
Requirement	Need or expectation that is stated, implied or obligatory. Requirements can be defined in
	terms of products, customers, organisation, regulatory or statutory.
Specification	Document stating requirements
Verification	Confirmation through the provision of objective evidence that specified requirements
	have been fulfilled.

- 58 Manning et al. (2019, p.1786) consider the weaknesses in current food assurance systems
- 59 stating:

60	"A failure to implement a systems-based approach [to assurance] means the use of private
61	standards will continue to be a shallow, rather than a deep form of implementation and
62	verification with associated limitations in the ability to deliver in terms of reducing the
63	likelihood of food safety incidents."
64	

- 65 Final product testing is not effective for food safety control and has instead been replaced
- 66 with preventative often systems based approaches to minimise the likelihood of food safety

67 incidents (Henson & Caswell, 1999; Zwietering et al. 2016). However product testing is part
68 of validation, monitoring and verification programmes that assure food safety and consistent
69 compliance with quality criteria within product specifications. The next section considers the
70 background to product testing in more detail.

71

2. Product testing

72 Product testing can be considered to be all the activities that measure or assess the 73 characteristics of a product or its component parts (ingredients, materials, packaging etc.) 74 Product testing is only of value if the sampling approach and associated sampling plans mean 75 that testing activities deliver results that are representative of the actual status of the product 76 and where the sampling plans are part of a wider food safety and quality management system 77 (Manning and Soon, 2018). Compliance can be determined as being the act of meeting multiple 78 requirements, standards, criteria and/or procedures that can be internally or externally defined 79 (Amundrud & Aven, 2015) and where required, independently verified. Alternatively, 80 compliance can be seen as:

81 "the act or status of complying with an imperative regulatory or normative requirement,
82 that is, compliance means working within boundaries defined by contractual, social, or
83 cultural standards (Manning, 2020, p. 995)."

84 Product compliance is assessed through multiple activities including product testing and these 85 activities can take place at a range of stages along the food supply chain from field to fork. 86 Product testing can be part of a hold (until compliance can be demonstrated) and release 87 programme often called positive release; or alternatively a negative release programme. A 88 negative release programme is where product is deemed to be compliant unless testing proves 89 otherwise. Some product testing has a lag phase until the results are received and this can add 90 cost to supply chains whilst results are awaited. Real-time positive release systems can provide 91 options for assessing the level of product compliance without this time lag, providing shorter

92 business cycle time, reduced inventories, improved process and product knowledge and 93 responsive analytical testing (Munir et al., 2017). Reliance on failure detection methods 94 especially if assurance systems are weak or have failed will lead to quality costs such as 95 rejection, disposal and potential fines for the failure to supply customers. In a just-in-time 96 supply chain, product testing has become secondary to process and documentation verification 97 with a focus on negative release systems for most quality aspects as they should have been 98 assured earlier in the process. However negative release systems do create a vulnerability point 99 for intentional substitution or adulteration to take place, because perpetrators know that their 100 actions will be largely undiscovered. Thus the potential for detection can act as a deterrence 101 strategy for food businesses.

102 **2.1 Food testing methods and rationale**

103 Costell (2002) outlines that any food testing methodology used in food manufacturing 104 and processing should follow a common approach and identifies two stages: the development 105 of the specification or quality standard and the development and validation of product testing 106 methods to ensure that the product, and its component parts can be tested appropriately to 107 ensure they comply with the quality standard and that the test itself is representative of the 108 material or product being tested. Materials, in-process materials and finished products can be 109 tested at multiple points from farm to retail shelf to ensure that they comply with the product 110 specification. Further assurance of complying with specifications may be provided with the 111 product e.g. a certificate of analysis or a certificate of conformity. These documents are 112 accepted along with the material on trust and are, if deemed appropriate, verified by customer 113 at a pre-determined frequency. For example, a manufacturer could purchase a set of spices 114 where the accompanying (paper or digital) certificate of conformity confirms that no sudan colours are present. The customer may not check the product, or may have developed a 115 116 sampling plan, based on assessment of the likelihood of the problem occurring, and will on a 117 routine basis verify that the sudan colours are indeed absent. As well as intrinsic product related 118 quality attributes being defined in specifications; specifications can also include extrinsic 119 process related claims (organic, animal welfare, sustainability related). Chain of custody 120 certification, especially with regard to sustainability related provenance claims is a well-121 established practice in value food chains (Mol & Oosterveer, 2015; Perales et al. 2019; Kayikci 122 et al. 2020). This means it is important to develop a supplier assurance protocol that includes 123 different activities to assure that suppliers have met specifications and procurement contractual 124 requirements, especially provenance where this is linked to a product claim. The stages are 125 now considered.

126 Stage 1.

127 The manufacturer, processor, retailer or brand owner needs to develop a specification or quality128 standard that describes the key requirements for the product. Specifications can include the:

Specification of food safety criteria (setting of critical limits) to ensure that the
 activities at a specified critical control point (CCP) within the manufacturing process
 are under control (Notermans et al. 1995);

 Specification of standards that can be are applied to products (product standards) and how those products are produced at each stage in the supply chain and how they are manufactured (process standards) see Henson & Caswell (1999). These standards Henson & Caswell argue can describe positive attributes i.e. characteristics or features that must be present in the product or process; or conversely negative attributes i.e. that should be prohibited, eliminated or reduced to a prescribed level in the product or process;

Specification of intrinsic criteria – an element of product standards that are defined
 for raw materials, part-processed and finished products. Intrinsic criteria covers

141 compositional and physicochemical characteristics and food micro structure that is142 present in food (Baka et al., 2016), and

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Contractual elements that relate to the contractual elements of the interaction between
 supplier and customer.

145 It is critical in the development of a specification that the requirements are complete enough to 146 ensure that the product complies with relevant legislation and market requirements but not so 147 cumbersome that it cannot be applied effectively in practice (Costell, 2002). For example, if a 148 retail product specification sets a standard for the cosmetic quality of tree matured apples, but 149 none of the suppliers can comply with the specification for colour, size or sugar content then 150 the retailer will either have no supply against that specification or will constantly be giving 151 derogations to the suppliers to supply at a lower specification. The specified product and 152 process attributes will also drive the cost of production. If there is a mismatch between the 153 standards specified, the price that the manufacturer is willing to pay, and the actual cost of 154 production will give rise to supply issues or be a driver for opportunistic behaviour.

155 **Stage 2.**

The second element is the development and validation of product testing methods to ensure they can determine in a reliable, repeatable and representative manner, if the product complies or does not comply with the specification requirements (Costell, 2002). Costello (2002, p.342) states that it is:

160 "not always the most precise and costly methods [that] are most suitable … the selection [of 161 product testing method] is based on the capacity of the method to measure variations in each 162 of the characteristics that influence product quality with sufficient precision [to demonstrate 163 that the product meets the specification].
164 Thus, the methodologies used for product testing must be able to demonstrate product integrity

165 for a given food.

166 **2.2 Product integrity**

Product integrity is the demonstration that for a given food, its innate characteristics can be reliably and repeatedly assessed with objective certainty. This is done by using analytical science methods which demonstrate that for a batch of raw materials, ingredients, or food, it contains all the component parts necessary to determine i.e. completeness (Manning & Soon, 2014). Alternatively, product integrity can described as the ability of a food, when tested, to meet an agreed specification, subject to the scientific confidence limits associated with the individual verification methods used.

174 The CEN Workshop Agreement (CWA) 17369:2019 Authenticity and fraud in the feed and 175 food chain differentiates between the terms authentic, authenticity and authentication (Table 176 2). Thus, a food product being determined as authentic is a status (Robson et al. 2020), that the 177 food product is what supply chain actors say it is, and there is an undisputable agreement 178 between the food product characteristics and the claims made about the food product (CWA, 179 2019). Thus, a characteristic is innate in the product itself and the claim reflects information 180 provided about the product in associated documentation, labelling, marketing information etc. 181 There are different kinds of adulteration that can occur including through adding, replacing 182 or diluting a given food (Table 2). The mixing or substituting of an inferior or foreign material 183 into a food is that it can be a food safety issue e.g. the adulterant can be a toxic or harmful 184 substance; it can reduce the innate nutritional quality of the food and/or affect the food in terms 185 of its utility i.e. affect its behaviour when it is combined with other ingredients, processed or 186 cooked. For example, diluting a batch of hard wheat, such as durum wheat, with soft wheats 187 affects the quality and utility of the resultant pasta and noodles when used (Kowalska et al. 188 2018) or using bleaching agents in wheat can prove to be a potential health hazard (Lohumi et al., 2019). 189

Table 2. Glossary of terms associated with authenticity and adulteration (Adapted from CWA, 2019)

Tarres	Definition
1 erm	Definition
Adulteration	A type of food fraud which includes the intentional addition of a foreign or inferior substance or element; especially to prepare for sale by replacing more valuable with less valuable or inert ingredients.
Authentic (food product)	A food product where there is a match [agreement] between the actual food product characteristics and the corresponding food product claims; when the food product actually is what the claim says that it is.
Authenticity	Not altered or modified with respect to expected characteristics including, safety, quality, and nutrition.
Concealment	Process of hiding the low quality of food ingredients or products.
Dilution	Mixing a liquid ingredient with high value with a liquid of lower value.
Food fraud	Intentionally causing a mismatch between food product claims and food product characteristics
Integrity (food product)	Genuine and undisputed in its nature, origin, identity, and claims, and to meet expected properties.
Substitution	Replacing a nutrient, an ingredient or part of a food often one with high value, with another nutrient, ingredient or part of food often one with lower value.
Unapproved enhancement	Adding unknown and undeclared compounds to food products in order to enhance their quality attributes.

193

194 So how would we categorise the innate characteristics of food?

195 2.3 The innate characteristics of food

196 The innate nature of food describes the ascertainable characteristics existing in, belonging 197 to or inherent in the food itself. The innate characteristics of plants, animals or synthetic 198 ingredients, sometimes termed intrinsic characteristics, can be defined in many ways. These 199 include:

199 Include.

200 (a) Describing foods in terms of the natural biomolecules they contain

201 These biomolecules include large macromolecules such as carbohydrates (polysaccharides), lipids, proteins or nucleic acids or small micro-molecules such as amino acids, 202 203 monosaccharides, fatty acids, nucleotides, vitamins etc. Biomolecules are usually produced by 204 the organism itself (endogenous) or taken up by the root system or eaten by the animal as an 205 essential nutrient (see also isotope analysis). Examples of essential endogenous biomolecules 206 are those biomolecules that cannot be synthesized by the organism e.g. certain amino acids. 207 Chromatographic analysis can be used to identify a range of food compounds and molecules 208 including peptides, carbohydrates, amino acids, fatty acids, additives, colourants, preservatives 209 which range from small to macromolecules (Danezis et al., 2016). Chromatographic 210 approaches can develop specific chemical fingerprints for each food using a range of 211 chromatographic techniques such as gas or liquid chromatography either as an individual 212 technique or combined with others specific to given food products. Vibrational and 213 fluorescence spectroscopy can also be used to determine the integrity of a food product against 214 a standard fingerprint using a range of spectral analysis. Within a written specification these 215 natural biomolecules will be defined in terms of the chemical properties of the food and also 216 the nutritional status of the food i.e. the biochemistry is described.

217 (b) Describing food ingredients in terms of being natural, nature identical and 218 synthetic ingredients.

219 Nature identical molecules or compounds are chemically synthesized to be replicas of the same 220 biomolecule that is found in nature. Examples of these food additives include flavours or 221 colours that are intentionally added to a food. Within the product specification of the food 222 product, these ingredients will be listed that are added to food e.g. nature identical carotenoids 223 added as a colourant to a drink or food to replace colour lost during processing. Synthetic 224 chemicals may also be intentionally added to food e.g. preservatives, colours, flavours, 225 stabilisers etc. that would not have been present in the food or its ingredients in the natural 226 state. Again, these would be defined in the specification and the ingredients list. This reflects 227 the food chemistry of an ingredient or composite food.

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(c) Describing the food in terms of sensory characteristics,

229 Sensory analysis is used to characterise the organoleptic characteristics of a food. Danezis et 230 al., (2016) identifies these characteristics as appearance, aroma, flavour, crunch and sound 231 associated with food and texture. Product testing involves the development of trained sensory 232 evaluation panels, but more recently emergent electronic noses (e-noses) and electronic 233 tongues (e-tongues) are being used in research. These have been used to determine the quality and innate characteristics of peaches (Xin, 2018); beer (Viejo et al. 2020) and olive oils
(Jolayemi et al., 2017; Buratti et al., 2018). The data derived from these techniques supports
the sensory attributes of the food.

237 (d) Describing the ingredients with a characteristic that relates to a variety, species or 238 breed,

239 Examples of these foods includes Angus beef, or basmati rice. Here the plant cultivars may be 240 from the same genus e.g. long grain rice, and basmati rice, but from different species or variety. 241 This is the same for when beef is sold as being from a certain breed (Genus Bos; Species taurus; 242 then multiple breeds e.g. Holstein, Angus, Hereford etc.) each breed will have a degree of 243 variability within the genome. Whilst whole genome sequencing (WGS) is of interest, it is the 244 development of specific genetic markers that also has been gaining focus. These genetic 245 markers can be used to identify fertility, production, disease resistance and carcase weights in 246 livestock. Single Nucleotide Polymorphisms (SNPs) are "nucleotide variations in the DNA 247 sequence of individuals in a population and constitute the most abundant molecular markers in 248 the genome." (Dadi et al. 2012, p28). These SNPs can link to quantitative trait loci (QTLs) 249 that will produce certain proteins and influence certain cellular functions, but will also identify 250 breed characteristics (Dadi et al. 2012). QTLs have been used to determine specific traits and 251 thus can highlight food fraud associated with Basmati rice (Kaur et al., 2015; Vemireddy et al., 252 2015). This field of science reflects the bioinformatic information associated with the food i.e. 253 the information associated with the molecular genetics and genomics of foods in totality or 254 ingredients. Bioinformatics draws together computer science, biotechnology, molecular 255 science and chemistry and the data derived reflects the genome of an ingredient or composite 256 food; or

(e) **Describing a food in terms of the proteins it contains.**

258 Proteomics is the characterisation of the whole set of proteins in an organism e.g. an animal or 259 a plant or a given part of that organism (fruit or seed, or organ of an animal). These proteins can be used as markers to define the innate characteristics of a food and the processes it has 260 261 been through e.g. to differentiate between liquid milk and reconstituted milk powder as the milk proteins in the milk powder will have been affected by the spray drying process. 262 263 Proteomics is the analysis of the complete proteome, or the total protein content of a particular 264 food or individual proteins and analysis of these proteins will inform on the properties of the 265 food in terms of analytical composition, food quality or origin of ingredients (Ortega et al. 266 2016). Ortega et al. (2016, p.212) state: "proteo- mics includes the structural and functional 267 knowledge of proteins [functional proteomics], but also the quantification of their abundance 268 [quantitative/differential proteomics], the study of their modifications, the interactions between them, and the study of their localisation [qualitative proteomics]." This work is of particular 269 270 interest when trying to isolate proteins using mass spectroscopy that in the susceptible 271 individual can cause severe allergic reactions (Korte & Brockmeyer, 2017; Monaci et al. 2018; 272 Marzano et al. 2020); presence of bacterial and chemical toxins (Gilquin et al. 2017) and to 273 determine food authenticity (Ortega et al. 2016; Korte & Brockmeyer, 2017). Advances in 274 mass spectroscopy and bioinformatics have meant that changes in the proteome that occur 275 during processing (cooking, drying, heating, and so on) can be determined in a food through 276 analysis (Mora et al. 2018). Examples of how these approaches can be used is to assess the 277 protein modifications between raw ham and cooked pork; pasteurised and unpasteurised milk; 278 meat quality in terms of tenderness, flavour, taste and consistency; fish quality and freshness; 279 potentially undeclared addition of certain plant material; identification of genetically modified 280 and non genetically modified foods (Ortea et al. 2016; Piras et al. 2016; Mora et al. 2018). Methods that support proteomics analysis include peptide profiling, protein profiling, peptide 281 282 mass fingerprinting, and use of eletrophoresis techniques (Ortea et al. 2016); Thus these activities reflect the proteome in totality or as protein fragments or peptides in a given food
product;

(f) Describing a food in terms of its provenance in terms of geographic location or source.

287 Provenance can relate to a particular geographic source or origin of a food and its individual 288 ingredients and/or relate to claims on how the product is produced and what claims have been 289 made about the product. More widely, provenance is described as relating not only to the place 290 where the ingredients and the final food are grown or caught, processed and finally 291 manufactured, but also aspects of how food is produced and if it is in line with prescribed 292 standard e.g. organic, halal and so on. Geographic indication has thus been linked to 293 provenance branding (Van Caenegem & Nakano, 2020), although proving that geographic 294 indication in practice can be difficult (Gangjee, 2017). Elemental and stable isotope 295 composition can be assessed in a given food to provide a chemical fingerprint including major 296 elements (Ca, Mg, Na, K), trace elements (Cu, Mn, Mo, I) and radioactive elements (Sr-90, U-297 234, U-238) where a specific profile can be linked to a given location (Kelly et al. 2005). 298 Isotopic and elemental fingerprinting has been used to characterise wines: trace element and 299 stable isotope ratio (Gonzalvez et al. 2009). Pepe and Vaccaro (2018) describe these major and 300 trace elements as a geochemical fingerprint which in terms of wine can link to the terroir 301 namely the interactive ecosystem of climate, geology, soil and plant and where plants are eaten 302 and converted to animal-derived food products too. Examples of elemental and stable isotopes 303 that can be use for geochemical profiling have been collated (Table 3)

Isotope abundances can vary with the geographic location, especially associated with soil or water composition that then influences the isotope composition in a given food. Geographic origin-based approaches utilise stable isotopes of elements such as carbon (C), hydrogen (H), nitrogen (N), oxygen (O) sulphur (S) or strontium (Sr) that vary in concentration

308 depending on the location of the food. (Wallace & Manning, 2020). An isoscape is the 309 "geographically patterned variation in isotopic compositions of a substrate as a function of 310 location, time (Bowen et al., 2009). The global water cycle and where precipitation falls will 311 vary in the heavy isotopes of H and O, the carbon cycle will also influence the ratio of carbon-312 13 to carbon-14 and the use of geographic information systems (GIS) can support the 313 development of an isoscape and local or regional isotope maps (Bowen et al., 2009). Isotope 314 maps have been developed for wine based on strontium (Durante et al. 2018), which will link 315 to underlying age of the rock in a location i.e. it is a geographic tracer (Kelly et al., 2005).

316	Table 3.	Examples	of geo	chemical	profiling	of foods
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Product	Geochemical profiling	Source
Bread	δ^{13} C, δ^{15} N, and δ^{18} O	(Suzuki et al., 2020)
Olives	δ^{13} C and δ^{18} O	(Chiocchini et al., 2016)
Onions	C, N, S, O, H, C/N, H/C, O/C, δ^{15} N, δ^{13} C, δ^{34} S, δ^{18} O, δ^{2} H	(Park et al. 2019)
Potatoes	$(\delta^{13}C, \delta^{15}N, \delta^{18}O, \delta^{34}S)$ and to element profiling (Na, Mg, P, S, Cl,	(Opatić et al. 2018a)
	K, Ca, Mn, Fe, Ni, Cu, Zn, Mo, Br, Rb, Sr), rare earth elements	
	(Sc, Y, Nb, La, Ce, Pr, Nd, Dy, Er).	
Rice	δ^{13} C, δ^{15} N and δ^{18} O	(Wang et al. 2020)
Tomato	major bioelements (δ^{13} C, δ^{15} N, δ^{18} O, δ^{34} S) macro and micro	(Opatić et al. 2018b)
	elements (P, K, Ca, S, Cl, Zn, Br, Rb, Sr), and chemical markers	
	(total antioxidant potential, total phenolic compounds, ascorbic	
	acid, lutein, nitrates and nitrites, ammonium).	

317

318 Isotope analysis can also be used to evaluate provenance claims for foods that relate to 319 production method or supply chain standards. Authentication of organic foods has received 320 attention as there are distinct practices which will affect the stable isotope profile of the food. 321 Agricultural practices e.g. the use of artificial or animal derived fertiliser will affect the ¹⁵N/¹⁴N 322 and sulphur isotope rations and the diets animals consume will affect the ¹³C/¹²C ratios (Kelly 323 et al., 2005; Inácio et al. 2015; Benincasa et al. 2018; Manning & Monaghan, 2019; Wallace 324 & Manning, 2020). In terms of provenance claims with fish stable isotope analysis can 325 distinguish between farmed and wild caught fish and seafood (Gopi et al. 2019a); but elemental profiling with seabass was said to be more accurate (Gopi et al. 2019b) and with multiple
methods (Varrà et al. 2019). Profiling techniques use a range of techniques such as Isotope
ratio Mass Spectroscopy (IRMS) and Nuclear Magnetic Resonance (NMR) see Danezis et al.,
2016). These analysis will identify the **origin** of the food.

This section of the chapter has considered the types of testing that can be used to determine the innate, intrinsic nature of foods, the next section considers the value of different aspects of testing in verifying food products.

333

3. Testing – where and how

Many of the methods described in this chapter are laboratory based, expensive to undertake and as a result would be used for verification rather than routine and general process based testing of food. However as technology evolves over the coming years, many localised, processed based solutions will evolve, especially if there is a market driver to ensure foods are authentic or free from contaminants.

339 Tests can be differentiated between destructive and non-destructive tests. For general 340 food quality testing non-destructive devices can be: firstly, laboratory based, stationary 341 equipment that us high cost but these are very precise and produces highly repeatable results. 342 Secondly, devices can be stationery sorting or grading equipment that is used in a processing 343 facility or sometimes as a field unit can use a range of inbuilt testing components e.g. colour 344 grading, size grading or cameras to identify defects (Musacchi & Serra, 2018). However, this 345 equipment can be is expensive to purchase and maintain. Thirdly, devices can be portable 346 and/or handheld devices, which are lower cost than off-line testing and may be less accurate, 347 but can provide real-time, rapid results (Ozaki et al. 2006; Salguero-Chaparro et al., 2013; 348 Abasi et al. 2018). A range of handheld equipment is being developed to determine innate 349 food attributes with non-destructive testing. These include handheld near infrared (NIR) 350 portable spectrophotometers for assessing adulteration of milk (de la Rosa-Delgado et al.,

2017); pork (Horcada et al. 2020); olive oil (Salguero-Chaparro et al., 2013) and oregano (McVey et al. 2020). Raman spectroscopy has been considered for in-container detection of counterfeit alcoholic drinks (Ellis et al., 2019) and handheld Raman spectroscopy devices for detection of milk powder adulteration (Karunathilaka et al., 2018). Studies have also considered how NIR combined with PLS calibration models can be used for nutritional attributes assessment (Neves et al. 2019).

357 Handheld e-nose systems are also being developed for food applications including rapid 358 and non-destructive testing for senescence in peach fruit (Wei et al. 2018), and beer quality 359 (Viejo et al. 2020), but the most progressive developments of e-noses are currently in the medical field. The reason for focusing on this aspect of food testing in the agri-food supply 360 361 chain is to consider both methods for on-line, real-time monitoring of the integrity of a food 362 product and off-line surveillance and verification methods that reflect wider systemic 363 approaches to producing and supplying materials and products that are safe and consistently 364 meet the agreed specification.

365 **4. Foodomics**

Foodomics is a wide field of science developed since the initial work of Cifuentes (2009) and this chapter has considered multiple applications in the advancing the field of analytical techniques to verify that products meet specification and product claims and also the authenticity of a food product or food ingredient. The concept of foodomics requires consideration of *the foodome* i.e. "the collection of all compounds present at a given time in any investigated food sample and/or in any biological system interacting with the investigated food." (Rychlik et al., 2017).

The foodome has been considered in this chapter as a subset of omics (see Rychlik et al. 2017;
2018) namely genomics, proteomics, isotopolomics and two further aspects are of note:
metabolomics, and metallomics,

376 The *food metabalome* is the metabolites present in a given food sample that can be 377 identified using targeted and non-targeted methods and techniques. Metabolomics uses the application of advanced scientific technologies, often associated with food science, computer 378 379 science and engineering science to identify the physical, chemical and biological structure of 380 food in order to determine the innate characteristics of the food and also its value in terms of 381 human health and well-being (Capozzi & Bordomi, 2013, p.1). Cubero-Leon et al. (2014) state 382 that the main advantage of metabolomics in determining the authenticity of a given food is the 383 untargeted nature of the analysis which supports the detection of emerging adulteration issues. 384 Developing product testing at the metabolomics level offers opportunities to connect a given 385 food to its metabolite profile or fingerprint, its innate quality traits, traceability criteria and the 386 location of origin (Uawisetwathana & Karoonuthaisiri, 2019). Metallomics is the study of the 387 interaction between bio metals, bio-function, and biochemistry within living things. 388 Metallomics considers interactions within a plant, animal, or food at the nanoparticle level. It 389 is an emergent discipline right now in food science but is set to develop further.

390 Foodomics is now being used in the assurance of quality, safety, and food integrity 391 within supply chains and also as a way to develop greater understanding of food biochemistry 392 (Munekata et al., 2020) and assist food manufactures and the medical profession to address 393 food nutrition and consumers' well-being and health (Andjelković et al. 2017), even 394 personalised nutrition. Foodomics requires a high level of data processing and as a result the 395 collection, analysis and management data is important as well as the development and use of 396 databases of a range of food profiles and metabolites (Jimenez-Carvelo, 2020). The technical 397 advances, especially around non-destructive on-line testing, can deliver increased sensitivity 398 and speed (Andjelković et al. 2017). Jimenez-Carvelo (2020) differentiate between the targeted 399 and untargeted approaches within the foodome (Table 4).

Table 4. Definitions of targeted and untargeted approaches within the foodome (Adapted from: Jimenez-Carvelo, 2020)

Approach	Description
Targeted	Based on the detection and quantification of a specific compound or a small group of compounds (metabolites or markers) present in the foodome. Within this approach is included the compositional analysis of profiles, knows as profiling where the goal is the identification and/or quantification of a set of related compounds which present structural or functional similarity, or because they are involved in specific metabolic nutritional pathways or offer a specific history for the product e.g. place of origin, variety, degree of freshness
Untargeted	Based on the analysis of unspecific instrumental signals without assuming any previous knowledge of relevant/irrelevant food components and it is represented by fingerprinting methodology. The sample foodome is considered as a whole rather than considering particular metabolites or compounds.

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Bigot et al. (2018) suggest that within the foodome as well as the development of food analysis
methods data management techniques will co-evolve such as multivariate analysis,
chemometrics, data mining and machine learning (Chaudhary et al., 2020).

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5. Concluding thoughts

This chapter has described the concept of product testing in agri-food supply chains and the methods that are being developed to identify instances of product non-conformance with either regulatory requirements, market requirements or both. The emergence of a range of new technologies provides opportunity to build on existing product testing protocols and offer complementary alternative and rapid testing of food which can provide assurance that food products are consistently what they are purported to be. Future advances could consider the right food at an individual, personalised level.

A personalised diet "requires matching human genotypic and phenotypic features to foods that increase the chance of achieving a desired physiological health outcome" (Gan et al., 2019, p.375). With the development of sequencing of the human genome, the rise of foodomics and the increasing knowledge about human metabolomics and food metabolomics, it creates a new context in which food specifications will be developed for the market, but increasingly at the personal level. 421 Smart food systems of the future will combine the data from existing and emergent 422 technologies along with the data that is generated through the supply chain. Effective and 423 targeted product testing acts as a potential deterrent against food safety incidents and food 424 fraud, and will assure product quality and compliance with specifications and contractual 425 requirements. However in the future, consumers (and consumers as athletes or patients) will 426 mediate the demands for safe food of the quality demanded at the price they are expected, and 427 willing to pay. The challenge will be how the food supply chain will maintain the supply of 428 affordable food, whilst embedding the technological advances that can and are deemed 429 appropriate to adopt. The biggest concern would be the development of a two-track food 430 system where one aspect of food provision will focus on reduced nutrient quality, limited 431 verification of safety and quality standards and operates through a least cost compliance 432 approach, whilst an alternative food provision is driven by high technology input, and high 433 integrity and transparency standards where the consumer is willing and able to pay a premium 434 for that level of assurance. The technical advances described in this chapter are ultimately 435 framed by a socio-political system that frames expectations and standards of safe abd quality 436 food.

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