

## Bibliometric insights into the Spectroscopy Research Field. A Food Science and

### Technology case study

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### Abstract

The food industry is in need of analytical solutions to maintain high quality and safety standards during the entire food production chain. Spectroscopy applications are targeted as a major solution due to its cost-effective, simple, efficient and multiparametric nature. Bibliometric studies provide a critical evaluation of the status of a research topic through the quantification of measurable outcomes of research activity. The main aim of this study was to use a bibliometric approach to the evaluation of the current status of the spectroscopy research applied to food science and technology. The critical evaluation of the results showed the most commonly used spectroscopy applications as well as the main attributes quantified. The bibliometric analysis also showed towards which food products the applications are directed. Intense research activity was observed for fruits, vegetables, cereals, meat, olive oil, water or wine. The use of near infrared in reflectance mode to non-destructively evaluate food quality was the main focus for most of the studies. Raman and fluorescence spectroscopy were also observed as frequently investigated techniques. Moreover, food adulteration, authentication, identification and quantification were the main applications reported. The incorporation of spectroscopy technology into food production processes is expected to progressively take place.

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**Key words**

Spectroscopy, food, non-destructive, quality, reflectance, bibliometric study

**Introduction**

The production of food by humans started due to the basic necessity of life. Since the very beginning food production has been facing the increasing challenges of food adulteration and counterfeiting. Food adulteration is defined as the lowering of the quality of food with potential health related problems of diverse nature<sup>1</sup>. Moreover, counterfeiting takes into account issues such as food produced outside specifications, registered methods or using unauthorized or expired ingredients<sup>2</sup>. Authentication of food products according to geographical origin such as wine or cheese<sup>3,4</sup>, meat adulteration<sup>5</sup>, the use of alternative fats and oils<sup>6-8</sup>, honey adulteration<sup>9</sup> or counterfeiting of milk and dairy products<sup>2</sup> are good examples of global food quality and safety challenges.

Ensuring high food quality standards has therefore become a priority for the food industry. High levels of food quality and safety are required in national and most importantly transnational food operations<sup>10,11</sup>. Process control strategies are thus necessary to ensure that quality and safety parameters are secured during the entire food production chain<sup>12,13</sup>. Process control strategies consequently need analytical tools to measure these parameters<sup>12,14,15</sup>. This applies not only to the food production process but also until food reaches the consumer at final destination (post-harvest)<sup>16</sup>. Spectroscopy applications are known by its accuracy, efficiency and often non-sample destructive nature and perfectly fit into the process control strategy<sup>17-19</sup>.

Traditional analytical methods have been employed over the past years to measure foods chemical composition and properties. A big effort is constantly being made to improve the accuracy and robustness of the analytical procedures but most importantly the required time of analysis. A big body of research is therefore directed towards the reduction of the analytical time, without compromising the accuracy of the measurements. However, despite the effort and constant progress some of the determinations still require time consuming protocols and advanced analytical facilities. The food industry is therefore in constant need of analytical alternatives ideally meeting the following specifications<sup>17,18,20</sup>. First of all, simplicity, rapidness

and cost-effectiveness are a must. Secondly, sample preparation needs to be reduced to a minimum or ideally completely avoided which in other words requires methods that are non-destructive<sup>21,22</sup>. Finally, the possibility to measure at-line, on-line or in-line is also becoming crucial for food industry practitioners<sup>20,22</sup>.

In spectroscopy applications, light is irradiated into the food sample using a variety of techniques<sup>23</sup>. Chemical information can thus be obtained when the outcome of the interaction of the light and the food sample is recorded. Spectroscopy calibrations correlate spectral data with chemical or physical information of the food sample. This information is obtained with the traditional reference methodologies. When the prediction models are properly calibrated and validated a highly accurate prediction algorithm is obtained and a single spectral measurement is the only requirement to quantify analytes or parameters of interest. Moreover, the development of these spectroscopy techniques have gone hand by hand with the progression of advanced chemometric tools<sup>4,19</sup>. Chemometric methods are mathematical approaches that extract the relevant information from complex data sets<sup>24</sup>. The progress recently made in the chemometrics field have boosted the appearance of spectroscopy calibrations relevant to a large number of food products<sup>25,26</sup>. The main benefits of these spectroscopy applications are therefore their easiness, robustness, versatility and multi-parametric nature as multiple parameters can be obtained from a single spectral measurement<sup>23,27</sup>.

Since the early development of spectroscopy applications in the food industry, a large variety of applications have been reported. Chemometrics tools were alongside developed and relevant information can therefore be extracted from complex spectral datasets. This has been utilized in a variety of food products and processes, including some of the most important food components such as fatty acids, oils, proteins or even phenolic compounds in wines and other food products<sup>20</sup>. In addition, spectroscopy applications have not only been used to quantify analytes but also to investigate relevant food properties. In this case, internal as well as external properties of fruits have been evaluated using different spectroscopy applications<sup>28</sup>. Apart from quantification purposes other uses have also been extensively explored such as adulteration or authentication of foods<sup>4</sup>. This was also possible thanks to the development of chemometric approaches through classification, discrimination or identification tasks<sup>4,19</sup>.

To be able to efficiently use spectroscopy applications, spectroscopy technology has simultaneously developed. For example, transmission spectroscopy is often used for liquid samples such as water, juices or alcoholic and non-alcoholic beverages<sup>27,29</sup>. Some of the probes have been developed in such a way that they can handle fermenting environments such as wine or beer fermentations. On the other hand, reflexion approaches are more suitable for solid samples, such as fruit or meat, or when internal or external properties are investigated<sup>20,28</sup>. Within reflexion techniques, attenuated total reflexion (ATR) offers the possibility to measure both solid and liquid samples<sup>30,31</sup>. Reflexion technology has gone even further and contactless instrumentation using reflected light is also available and potentially suitable for other applications<sup>20–22</sup>. The relevance of contactless technology opened up the possibility to evaluate food processes, such as for example when food samples are transported through the process line or pipe in the case of liquids or through a moving conveyor in the case of solid samples<sup>21</sup>.

The technology currently available is therefore providing a variety of applications that can be used off-line (after sampling, spectral collection takes place in a laboratory), at-line (when instrumentation is placed close to the process line), on-line (through and automated sampling system) and also in-line (spectral data is collected in situ from the sample during the process)<sup>20,22</sup>. Applications have thus been reported in a variety of food products such as meat and meat products, seafood, milk and dairy products, fruits and vegetables, grains and related products, water and wine<sup>20</sup>. The possibility to measure chemical and physical information from food processes is obviously paving the way towards the implementation of process monitoring and process control strategies leading towards process optimization to ensure food quality and safety<sup>17,18,20,22</sup>.

The capabilities of spectroscopy applications make them very attractive for the food industry as it provides a simple and inexpensive way to monitor quality standards. The progressive implementation of this technology into food production chains has been observed over the past years<sup>20</sup>. It is also foreseen that more and more applications will become part of the food production chain in the near future. The main aim of this study is therefore to perform a bibliometric evaluation of the current status of the spectroscopy research applied to food science and technology. Bibliometric studies employ quantitative methods to critically evaluate research outcomes as well as present and future research trends<sup>32</sup>. Despite the

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3 122 increasing importance of spectroscopy in food applications, this will be, to the authors  
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5 123 knowledge, the first bibliometric attempt to evaluate the research status of spectroscopy  
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7 124 applications in food production.

## 8 9 125 **Materials and methods**

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12 126 The following search strategy was used to obtain the records evaluated in the present study:  
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14 127 Title = (spectroscop\* OR spectrophotometr\*). The quantitative data was extracted from the  
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16 128 Web of Science Core Collection (WOS) database from Clarivate Analytics. The search was  
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18 129 restricted to the articles published under the Food Science and Technology subject category.  
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20 130 Moreover, the search was conducted in the title field with the aim of minimizing the inclusion  
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22 131 of non-relevant results, therefore increasing the accuracy of the search strategy. Both terms  
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24 132 were truncated with an asterisk to include the derived words originating from the word roots.  
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26 133 For example, the root spectroscop\* can lead to spectroscopy or spectroscopic. The  
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28 134 bibliometric search was limited to the last 10 years covering the period between 2009-2018.  
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30 135 Peer-reviewed research papers such as articles and reviews were the only records included in  
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32 136 the study. Proceeding papers, notes, editorial material, corrections and abstracts were  
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34 137 therefore excluded. Before key word analysis was attempted, a key word standardization task  
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36 138 was performed. Acronyms, derivations of the same terms, spelling variations and synonyms  
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38 139 were therefore standardized.

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40 140 Bibliometric studies follow a quantitative approach to evaluate the scientific performance of  
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42 141 a research topic. The papers evolution during the years of the study, most prolific institutions  
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44 142 and countries, the most included author's keywords and the subject categories, as defined in  
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46 143 the WOS, were evaluated as indicators of scientific production. Bibliometric studies also aim  
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48 144 at evaluating the scientific impact. In this study, number of citations per article, journal impact  
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50 145 factor and quartile were used as indicators of scientific impact. This information was obtained  
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52 146 from the Journal Citation Reports (JCR) last available report (2017) at the time the records  
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54 147 were extracted.

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56 148 Social network analysis (SNA) provides a representation network of the relationships between  
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58 149 quantitative and qualitative data. SNA makes use of node entities (spheres) and ties  
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60 150 (connecting lines) to measure and map complex network relationships between information  
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152 containing entities (institutions, countries or keywords in this study). Social network analysis  
was used to evaluate collaboration patterns between institutions or countries through co-

occurrences in published papers<sup>33</sup>. In addition, the keywords assigned to the papers were also analysed through subject analysis. The frequency of inclusion and the co-occurrence between two words were evaluated. The co-occurrence indicates the number of times a pair of words is repeated. Institutions and countries collaborations and key word analysis are represented in network graphs. The strongest associations are thus easily visualized. Pajec and VOSViewer software is used for network representation<sup>34</sup>. To improve network visualization a minimum of publications (threshold) is applied for keywords, institutions and countries co-occurrences. For the key word analysis, the size of the spheres indicates the number of publications containing a keyword, whereas the thickness of the lines provides the number of co-occurrences between two keywords. In the case of institutions and countries, the line's thickness indicates the intensity of the collaborations and the spheres' size the number of publications in the corresponding institution or country for the topic under study.

## **Results and discussion**

Bibliometric studies provide a quantitative evaluation of the scientific production and impact of a research topic. These studies also provide improved understanding of the scientific structure of the topic of interest, including the potential identification of current and future trends. This is done in the form of keyword analysis and through the identification of research collaborations. Valuable information is therefore provided for new and existing researchers. Bibliometric studies have been published in areas as diverse as: plant genetics<sup>35</sup>, biotechnology<sup>36</sup>, biomass and bioenergy production<sup>37</sup>, food and food safety<sup>38</sup>, viticulture and oenology<sup>39,40</sup>, soil contamination<sup>41</sup>, deforestation or climate change<sup>42–46</sup>. However, despite the relevance of the topic, a bibliometric study covering the spectroscopy research applied to food science and technology has never been attempted before.

The term spectrophotometry is often used when ultraviolet and/or visible light is the source for spectral measurements<sup>47</sup>. Due to the importance of this technology, to quantify certain analytes characteristic of food samples, it was decided to include this term and therefore prevent the potential exclusion of relevant records. In a similar fashion, the word spectrometry could have also been included, however the term is strongly associated with mass spectrometry, term that falls outside the scope of spectroscopy applications, being therefore in this case not included.

Since the early developments of spectroscopy applications during the 1970s a steady increase in the number of publications was observed (data not shown). Initially, up until the 1990s the increase was quite moderate. After this period a more intense increase was observed. However, it is not until the first decade of the twentieth century when an exponential increase in the number of publication was highlighted. This increased interest in the topic can be associated to not only the development of chemometric tools and software capable of dealing with more complex sets but also to the higher demand of food quality and safety standards nowadays required for food products. Due to the fast development in the field observed in recent times, this article focusses exclusively in the last exponential growth period.

**Annual evolution of articles and citations received.** Figure 1 shows the number of published records as well as the number of citations for the 2009-2018 period. A total number of 3142 papers were published within this period, with the published articles receiving a total number of 37078 citations. An increasing trend in the number of publications from 2009 until 2017 (last year with completed number of articles) can be depicted. Within this 10 year's period the number of published papers have doubled (200 papers in 2009 to > 400 in 2017), showing the progression and development taking place in this field of research. In terms of number of citations, 2011 appeared as the year with the highest number. After 2011, a plateau that lasted for three years followed by a decrease in the number of citations was observed. The citation patterns do not follow the increasing trend observed for the number of articles. The reason for this behaviour could be assigned to time, as more realistic citation counts are observed after some time since publication took place. If the ratio citation per paper is normalized with the number of years since publication, a very similar ratio around 2.5 is observed until 2014, with a subsequent decrease until 2018 that might be attributed to the time factor mentioned earlier.

**Most prolific journals.** The most prolific journals are summarized in Table 1. The number of publications and citations, the ratio citations/publication, the impact factor of the last 5 years as well as the WOS subject category and quartile are also represented. A threshold of 40 publications in the period under study was applied. The two most prolific journals appeared to be *Food Chemistry* and *Analytical methods* with over 450 papers. In third place, *Journal of Agricultural and Food Chemistry* appeared with more than 250 papers. The following journal with nearly 200 papers was *Food Analytical Methods*. *Journal of AOAC International* and

*Journal of Food Engineering* were also found as prolific journal with 100 publications. Interestingly, for three out of six journals a strong focus is placed on the development of analytical methods, while the other three cover a variety of research topics, non-exclusive of analytical procedures. Table 1 also showed that *Journal of Agriculture and Food Chemistry* displaces *Analytical methods* as the second most prolific journal in terms of citations. This is further confirmed when the ratio citation per article is evaluated. The ratio citations per paper provides a better indication of the impact of a journal for a specific topic, spectroscopy in this study. This is because only the citations received by papers in this field of study are considered. The journal with the higher impact (citations/paper) was *Food and Bioprocess Technology* (24.41), followed by *Food Research International* (23.14) and *Meat Science* (20.22). After this trio of journals, two of the most productive journal showed also high impact i.e. *Journal of Agricultural and Food Chemistry* (19.73) and *Food Chemistry* (18.65). In terms of impact factor in the last five years according to the JCR, *Food Chemistry* (4.946) appears once more as the leading journal followed by *Food Research International* (4.196), *Food Control* (3.891), *Journal of Food Engineering* (3.851), and *Journal of Agricultural and Food Chemistry* (3.791). Surprisingly those journals with implicit focus on methods development showed lower impact factor as well as lower ratio citations/paper. On the other hand, England and specially USA are responsible for the management of the journals in the field, with the only exception of *Postharvest Biology and Technology* journal, placed in the Netherlands. Finally, as expected, *Food Science and Technology* was the preferred subject category followed by *Chemistry*, *Analytical* and agriculture related categories. This indicates firstly the relationship between food science and agriculture and secondly the inclusion of spectroscopy applications as a measuring tool for food analysis. Most of the journals are included within Q1, with again journals orientated to the development of analytical methods often appearing in Q2 and Q3.

**Most cited papers.** Papers with more than 100 citations are listed in Table 2. Only two papers were found above 200 citations. The paper with the highest number of citations (246) was published in collaboration between the Water Research Centre in Australia and three institutions in Denmark. This tutorial review article was published in *Analytical Methods* journal in 2013 and exposes a tutorial review on the use of multi way techniques and fluorescence spectroscopy<sup>48</sup>. The article refers specifically to parallel factor analysis



(PARAFAC) used to decompose tri-linear data sets such as those arising from excitation emission matrices (EEM) of fluorescence applications. This paper also stands out in first position when the number of citations is standardized with the number of years since publication, which serves as an indication of its scientific relevance and impact. The second most cited paper reviews the near infrared reflectance applications to predict meat and meat products quality<sup>5</sup>. The paper was a collaboration between three institutions from three different countries i.e UK, Spain and Australia. Interestingly, the authors mentioned the poorer ability of this technology to predict technological and sensory characteristics of meat. However, chemical properties or quality grades classification are accurately predicted. Moreover, the need to better understand the wavelength regions within the NIR spectra associated with the meat quality is pointed out. This will potentially lead to more accurate calibrations and also to develop customized technology for this type of applications. When the standardized number of citation is evaluated, a very similar ratio was observed (just under 20) for the top 11 articles with a slight decrease for the remaining publications included in Table 2. Among them, a paper with a standardized ratio of 22 stood out. The publication reports a review article on the application of surface enhanced Raman spectroscopy (SERS) for food safety<sup>49</sup>. The article emphasizes on the role of SERS to evaluate pathogenic microorganisms, food contaminants and food adulteration as main applications for this technology.

**Institutions collaboration.** Seventy networks were obtained from the social network analysis, spanning from 2 partners to 23 institutions networks. The collaboration threshold was set up at 2 collaborations. The four bigger collaboration networks obtained are shown in Figure 2. The first and most prolific collaboration network includes in its entirety French institutions, with Unite Mixte the Rechercher (UMR) and Institute National de la Recherché Agronomique as the leading institutions. The second collaboration network contains USA institutions with the United States Department of Agriculture (USDA) playing a central role. International partnership is also observed in this network with some prolific collaboration with Chinese institutions, with the Chinese Academy of Agricultural Sciences (CAAS) as the most prolific. The third collaboration network is a combination of Chinese and Irish institutions with the University College Dublin playing a central role with solid collaborations with the National University of Ireland and Food Refrigeration and Computerized Food Technology (FRCFT) also

in Ireland. The most prolific Chinese institutions were in this case: South China University of Technology, Zhejiang University, Engineering and Technology Research Centre Guandong and Guangzhou Higher Education Mega Centre. Finally, the fourth collaboration network includes mostly Argentinian research institutions with the Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) as most prolific institution. Institutions from Italy and Brazil were also observed in this collaboration networks.

**International collaboration.** The strongest collaboration was observed between China and United States (Figure 3). The second most prolific collaboration was found between Malaysia and Indonesia, however with a lot less intense collaboration than USA and China. China with Canada and Ireland also showed prolific collaboration activity. Strong collaboration activity was also observed for some European countries. However, the intensity of the collaborations is distributed between a larger number of countries as no strong individual collaborations were observed (thinner connecting lines but large sphere size). This is the case for United Kingdom, German, Italy or Spain. Brazil or Australia also appeared as countries with intense collaboration activity. In the case of France, that showed a strong internal collaboration activity in the institutions analysis, a smaller international collaboration intensity can be depicted from the thickness of the lines and slightly lower research productivity from the size of the sphere.

**Key word analysis.** The keyword network was extracted using 45 co-occurrences as threshold. Figure 4 showed the collaboration network with 73 words included. The expected central role of the word *spectroscopy* is accompanied by an inner ring of keywords that includes in first place, and based on the size of the spheres, *near infrared* and *infrared*. With a much smaller presence, the key words *Raman*, *mid infrared* and *visible* appeared also as part of the inner ring, whereas a smaller presence was observed for *ultraviolet*, *nuclear magnetic resonance (NMR)* or *fluorescence*. It thus seems that near infrared is the predominant region employed in spectroscopy applications developed for food products. The keywords *Fourier transform*, *chemometrics* and *partial least squares (PLS)* also stood out sharing strong links with spectroscopy. The use and development of chemometric tools took place alongside with the development of spectroscopy applications for the food industry. The spectral data need to be correlated with chemical information characteristic of the food being evaluated. PLS is observed as the most widely used and successful technique to correlate both data sets. This

technique is mostly used for quantification purposes as can be observed with the links between *partial least squares (PLS)* and the keyword *quantification*. The word *prediction* was also identified in the keyword network. The use of this term might be due to the nature of *spectroscopy* applications where an indirect *quantification* based on spectral information is provided i.e. a *prediction* is provided. Moreover, the inner ring also contained the main *chemometric* tasks using *multivariate data analysis* performed in spectroscopy applications i.e. *quantification*, *classification* and *discrimination*. Interestingly the keyword *reflectance* was also widely used, indicating the suitability of reflexion spectroscopy in food production, ideally used for *non-destructive* and *rapid analysis* during the food production process. The final purpose of using spectroscopy applications is to optimize product *quality*, which might explain the strong presence of this later keyword. Finally, the keywords *adulteration*, *identification* and *authentication* were also identified providing evidence of the most common applications spectroscopy is used for. Other words with an important role on the chemometric treatment of the data were *principal component analysis (PCA)*, *partial least square discriminant analysis (PLS-DA)* or *support vector machines (SVM)* as well as the keyword *variable selection*, indicating the importance of identifying the information containing regions within the *spectra*.

**Individual evaluation of food products.** With the objective of a more detailed evaluation of specific food products, a keyword analysis as well as the identification of the most cited papers were undertaken. From the keyword network a number of food products relevant to the topic were observed (see Figure 4). These included: olive oil, meat, fruit, milk, apple, pork, beef, wheat, cheese, wine and water. The identification of the most frequently used keywords for the specific food products and the discussion of the most cited papers will provide a critical evaluation of the status of the spectroscopy research with a sole focus on an individual food product. Table 3 shows the first 20 keywords in order of appearance that co-occurred with the corresponding food product. The highest co-occurrence was always with the word *spectroscopy* and the number of co-occurrences with this word is included in brackets following the food product. Moreover, Table 4 shows the most cited papers for each food product, authors, journal, publication year and number of citations.

Common words repeatedly observed included some of the most used keywords as identified in the keyword network (Figure 4). Keywords such as *infrared*, *chemometrics*, *Fourier*

transform, spectra, multivariate data analysis, partial least squares regression (PLS) and food were commonly represented. However due to its minor significance towards the spectroscopy applications of the different food products, the above-mentioned keywords will not be further discussed.

Olive oil. The most widely used keywords for olive oil were *authentication* and *adulteration* which pointed out the main issues that the olive oil industry is facing. The *adulteration* of olive oils with lower quality oils or oils from other botanical origins is very often reported. On the other hand, the best producing regions have also taken measures to protect growers and consumers with a large number of studies evaluating different *authentication* strategies. This links with other key words such as *classification* and *discrimination*, statistical terms used in *adulteration* or *authentication* tasks. In addition, the appearance of the keywords *edible oils*, *vegetable oils*, *fatty acids* and *phenolic compounds* highlights these components as the ones most commonly measured when oils are evaluated. Finally, in terms of the spectroscopy techniques used, *Raman* spectroscopy was the most commonly used keyword followed by *near infrared*. *Nuclear magnetic resonance*, *fluorescence* and *mid infrared* spectroscopy applications would also be commonly used to evaluate olive oil samples.

The most prolific paper was published by a Spanish group in *Food Chemistry* in 2010. This study evaluated the suitability of Fourier transform infrared spectroscopy (FTIR) to authenticate vegetable oils of different botanical origin and to establish the composition of binary mixtures with other edible oils (Table 4). The results showed the suitability of this spectroscopy application to authenticate and detect the presence of other oils<sup>50</sup>. The second most prolific paper, also published in 2010, also makes use of FTIR and evaluates the adulteration of olive oil with palm oil<sup>51</sup>. This paper was a collaboration between two Malaysian and Indonesian institutions, and serves as an example of what was observed in the international collaboration network. The percentage of palm oil was accurately predicted from the FTIR spectra. Moreover, a discriminant analysis led to the successful classification of adulterated and olive oil samples. The third most prolific publication with more than 100 citations monitors the fatty acid content in virgin olive oil from attenuated total reflectance (ATR) FTIR spectra using partial least squares regression (PLS)<sup>52</sup>. This paper is also an example of international collaboration between Italy and Argentina, published in 2009 in *Food Chemistry*. The remaining publications with less than 100 citations are in line with some of

the most used keywords such as near and mid infrared, fluorescence, authentication or adulteration.

Fruits. The first four most commonly used key words provide a clear overview of the spectroscopy exercises undertaken for fruit products. *Near infrared* in *reflectance* mode to perform a *non-destructive* evaluation of fruit *quality* would be the requirements for spectroscopy application in fruits. The importance of spectroscopy approaches in *apple* fruits is identified from its higher position within the most commonly used keywords. Interestingly the keyword *vegetables* is also frequently used which points out similar spectroscopy requirement when evaluating these particular food products. Other relevant keywords refer to some of the fruit properties quantified as it is the case for *soluble solids*, *firmness*, *antioxidants* and *sugar content* or *phenolic compounds*. Finally, it is also important to mention the presence of *visible* spectroscopy, most probably for colour evaluation of fruits and vegetables and *storage*, indicating the importance of postharvest technology applications making use of spectral measurements.

The most cited article, with more than 100 citations, studied the suitability of NIR spectroscopy to evaluate postharvest quality through brix degrees and firmness in apple fruits<sup>53</sup>. The authors concluded that to obtain robust calibrations the models needed large data set containing sufficient relevant variability in terms of seasons, origins, cultivars and storing conditions. This paper, published in 2010 in *Postharvest Biology and Technology*, was obtained from an international collaboration between Belgian and Romanian institutions. The second most prolific paper with 87 citations was published by researchers at the Australian Wine Research Institute in Food Research International. The article presents a tutorial to evaluate model performance in spectroscopy applications with a specific focus on fruit and fruit juices<sup>19</sup>. The versatility, effectiveness and multi-parametric nature of spectroscopy applications are highlighted in the study<sup>19</sup>. In third place appeared a study using VIS/NIR in reflectance mode to quantify soluble solid content, pH and firmness in pear fruits<sup>54</sup>. The paper was published by a Chinese research group in *Journal of Food Engineering* and focusses on alternative chemometric tools to improve model performance with the use of non-linear supporting vector machines (SVM) algorithm and variable selection tools based on effective wavelengths according to regression coefficients. Non-linear regression methods are proposed as a valid alternative to evaluate internal properties of fruits<sup>54</sup>.

401 Apple. In the case of spectroscopy applications on apple fruits a different keyword preference  
 402 was observed. *Near infrared* appeared as the most commonly used key word and as the  
 403 technique of choice. *Visible* spectroscopy is also represented possibly pointing towards fruit  
 404 colour. Secondly, words such as *reflectance* or *diffuse* indicate the most common approaches  
 405 used to evaluate apple *quality* and more specifically *internal quality*. Other important  
 406 attributes are *firmness*, *soluble solids*, *sugar* and *dry matter*. The word *storage* indicated also  
 407 the importance of spectroscopy applications in postharvest technology. Finally, it is also  
 408 important to mention the presence of the keyword *non-destructive*, indicating the nature of  
 409 the applications needed for the quality control of apple fruits.  
 410 The most prolific paper coincides with the one observed for fruits and as mentioned deals  
 411 with the suitability of NIR spectroscopy to evaluate postharvest quality in apple fruits<sup>53</sup>. The  
 412 second most prolific publication was published in *Food and Bioprocess Technology* in 2013  
 413 from a collaboration between China and USA. The paper makes use of surface enhanced  
 414 Raman spectroscopy (SERS) to detect pesticides in fruits<sup>55</sup>. The value of using SERS relies on  
 415 the ability to enhance the sensitivity of traditional Raman spectroscopy, normally used to  
 416 measure compounds found at higher concentrations<sup>56</sup>. The detection and quantification of  
 417 food contaminants and adulterants are some of the most relevant applications of SERS<sup>56</sup>. This  
 418 technique although promising does not meet the non-destructive nature of most of the  
 419 applications reported for apple and other fruits. Other publications with high citation counts  
 420 also made use of SERS technology to evaluate the presence of residues in apples. Moreover,  
 421 sensory and chemical evaluation of apples using non-destructive methods were reported to  
 422 quantify vitamin C, phenol compounds, soluble sugars, antioxidant capacity or sensory  
 423 attributes.  
 424 Meat. *Near infrared* in *reflectance* mode to evaluate meat *quality* appears to be the technique  
 425 of choice for these food products. Moreover, *beef* and *pork* seems to be the focus in meat  
 426 applications with specific emphasis in *muscle*, *water holding capacity* and *chemical*  
 427 *composition* measurements. *Raman* spectroscopy is also highly positioned indicating the  
 428 suitability of this technique for meat evaluation. *Adulteration*, *authentication* and  
 429 *identification* seems to be a priority for meat applications with the corresponding *prediction*,  
 430 *classification* and *discrimination* tasks.

The most cited article with more than 200 citations was a review paper published from a collaboration between the UK, Spain and Australia in *Meat Science* journal. The focus of the paper is placed on infrared reflectance spectroscopy applications for meat and meat products quality prediction<sup>5</sup>. Interestingly the authors highlighted the suitability of these techniques to accurately predict a large number of chemical meat properties but lower ability to estimate technological and sensory attributes<sup>5</sup>. Sample heterogeneity, reference methods performance and subjectivity of sensory evaluations are suggested as the main reasons. On the other hand, successful categorization of meat into quality classes was also observed in this review paper. The second most published paper from a research group in China received 87 citations. The study evaluates the suitability of reflectance FT-NIR for the quantification of total volatile basic nitrogen (freshness) and the Warner-Bratzler shear force (tenderness) in pork meat<sup>57</sup>. The authors highlight the real time and at-line nature of the application with potential improvement of quality control of pork meat. The third most cited paper evaluates the suitability of fluorescence spectroscopy to evaluate protein oxidation markers in meat products. Although a spectroscopy calibration per se was not used in the study the potential of fluorescence spectroscopy to evaluate oxidation markers was highlighted<sup>58</sup>. This paper also published in *Meat Science* journal showed a successful collaboration between Finland and Spain. Other identified topics covered meat adulteration exercises, lamb and chicken applications or protein quantification in meat products.

Beef. As observed for meat, *NIR* spectroscopy in *reflectance* mode to evaluate beef meat *quality* seems to be the main research focus. In addition, *Raman* and *fluorescence* are also represented within the most used keywords. Fatty acids, colour, tenderness and chemical composition are the most common attributes investigated with the development of calibrations for *quantification* and *prediction* purposes. The word *muscle* show that reflectance spectroscopy is widely applied directly into muscular tissue or applications on direct *muscle* measurements are desired. Finally, *adulteration* tasks seem to be the priority in this case. Interestingly, the word *pork* has been also associated with beef as similar applications might apply to both meat types.

The most prolific article was published in *Food Chemistry* and shows a novel approach using Raman spectroscopy to discriminate beef and horse meat. After an extraction process of the fat content of the samples, an accurate discrimination of adulterated samples was achieved<sup>59</sup>.

The second study with the largest number of citations shows a collaborative work between three institutions in the UK. The article investigated reflectance visible-NIR spectroscopy to predict chemical physical and sensory properties of beef quality<sup>60</sup>. Attributes such as colour, cooking loss, instrumental texture and sensory characteristics were evaluated. The results, in agreement with previous studies<sup>5</sup>, showed that VIS-NIR is able to accurately predict colour properties but did not perform for sensory attributes, cooking loss and instrumental texture. The importance of including relevant variability in the sample set is also highlighted by the authors of the study. Identification tasks of different meat types, authentication of adulterated meat, fat content quantification, meat spoilage issues or consumer studies were also represented.

Pork. In agreement with meat and beef the keywords *near infrared*, *reflectance* and *quality* are the most widely used. In this case the most important properties seem to be *water holding capacity*, *colour*, *fatty acids* and *sensory analysis*. *Muscle* and *early post-mortem* are indicating when and in which tissue are the measurements taking place. *Prediction* and *classification* are the preferred task for this meat product. Moreover, *Raman* spectroscopy has also been explored as can be depicted from his inclusion in the most widely used keywords. The word *beef* was also found relevant an as mentioned most probably due to similar applications in both meat products.

The most and third most prolific papers coincides in this case with those observed for meat. The first one corresponding to the review article on the use of NIR to predict meat and meat products quality<sup>5</sup> and the third one to the evaluation of tenderness and freshness in pork meat using FT-NIR<sup>58</sup>. The second most prolific paper reports on the suitability of ATR-FTIR to evaluate adulteration of beef meat balls with pork meat. This paper is a collaboration between several Indonesian and Malaysian institutions and was published in *Meat Science* journal in 2011. From the reported results FTIR was showed as a valid approach for the detection and quantification of pork meat in beef meatballs<sup>61</sup>. Discrimination of pork storage, sensory prediction of pork meat or pork meat adulteration were topics widely covered. Some of the most important attributes were water holding capacity or fatty acid content of pork meat.

Milk. *Near infrared*, *fluorescence*, *mid infrared* and *Raman* were found in this order as some of the most widely used keywords. These results indicate a wide variety of techniques been



applied to milk with the appearance of the keyword *reflectance* pointing towards the suitability of this spectroscopy approach. *Adulteration* of milk seems to be a relevant topic, with *authentication* also been observed. Moreover, *proteins* and *fat* are the two most common researched attributes. *HPLC* and *tandem mass spectrometry* are the analytical techniques most commonly employed to generate the reference data. Other words such as *dairy products* and *cheese* are also observed indicating an extended use of spectroscopy applications in milk derivatives.

The article that received the largest number of publications was published in the *Journal of Agricultural and Food Chemistry* in 2009 from a collaboration of two German institutions. The paper evaluates the suitability of NMR spectroscopy to identify melamine contaminated infant formula dissolved in liquid samples and concludes that spectroscopy can be successfully used for quality control and food safety<sup>62</sup>. The second most prolific paper was published by a group of researchers from India in the same journals. In this case fluorescence spectroscopy was used to evaluate the stability of curcumin and *beta*-Lactoglobulin aggregates. The decrease in solubility of the complex enables the use of curcumin for therapeutic purposes<sup>63</sup>. The third most prolific publication appeared in the *Journal of Dairy Science* from a collaboration between Ireland and Italy. Mid infrared spectroscopy is used to predict coagulation properties, titratable acidity and pH in cow's milk. The results showed MIR spectroscopy as a promising technique to quantify rennet coagulation time, titratable acidity and pH with the authors also pointing out that models need further development<sup>64</sup>. The analysis of fat composition and protein, milk adulteration or the detection of milk origin were some of the most commonly observed topics.

Cheese. In agreement with milk, *near infrared*, *fluorescence*, *mid infrared* and *nuclear magnetic resonance* are the spectroscopy techniques identified in cheese applications. *Fatty acids* and *proteins* are the components of interest analysed to evaluate cheese *quality* making use of *HPLC* analysis. *Authentication* tasks using *discrimination* analysis are widely used to evaluate *geographic origin*.

The most prolific publication studied the discrimination between local and foreign milk samples for mozzarella cheese production<sup>65</sup>. In this case nuclear magnetic resonance was used in combination with other analytical techniques to attempt the discrimination between milk samples. This paper published in *Food Chemistry* is an example of international

collaboration between Italy and Slovenia. The results highlight fatty acids as the components with higher discrimination ability<sup>65</sup>. NMR also provided valuable data in the sense of sugars, amino acids and organic acids. The coagulation properties of milk are in this case one of the most reported topics. Spectroscopy application to quantify mineral content, sensory attributes and peptides were often reported. Moreover, authentication and geographical or milk origin studies were also frequently reported

Wheat. Commonly to other food products, the most commonly used words were *near infrared*, *reflectance* and *quality*. *Nuclear magnetic resonance (NMR)*, *Raman* and *fluorescence* spectroscopy applications have also been researched for wheat applications as suggested by the frequency of use of these keywords. The appearance of the keyword *transmittance* is also suggesting the use of this approach to quantify wheat properties. Moreover, the words *plants*, *grain*, *kernels* and *barley* indicate the focus of the applications. *Proteins*, *moisture* and *starch* were identified as the measurements of interest for wheat applications.

The most cited paper was published in the *Journal of Agricultural and Food Chemistry* in 2010 and investigates the suitability of NIR reflectance spectroscopy to predict protein, starch and seed weight in seeds. The authors concluded that NIR spectroscopy could be used to accurately sort seed traits with no sample preparation<sup>66</sup>. The second most prolific paper attempts to discriminate wheat geographical origin again using NIR reflectance spectroscopy. Several chemometric discrimination tools were evaluated with different classification ability as indicated by the authors<sup>67</sup>. The third most prolific paper presents a novel approach to analysis of wheat grains<sup>68</sup>. This scientific contribution was published by a group of French researchers from two institutions. In this case laser induced breakdown spectroscopy is used to evaluate elemental composition on grains. The article evaluates structural analysis of vegetal material through a classification exercise.

Water. A different keyword profile was in this case observed. Interestingly, and for the first time, the word *food* appeared as the most commonly used keyword. *Near infrared* was also one of the most frequently used keywords. Other spectroscopy applications included *spectrophotometry*, *atomic emission spectrometry* and *nuclear magnetic resonance (NMR)*. The keyword *reflectance* was also observed in agreement with the other food products. *Chromatography* and *HPLC* are suggested as the preferred analytical techniques. The key

word *preconcentration* appeared as one of the most frequently used, probably due to the low levels of compounds quantified in water samples, needing of this step before evaluation. This is in line with the key word *extraction* and the separation technique *cloud point extraction*. The evaluation of *moisture* content in other products such as *meat* to evaluate product *quality* was also represented in the most frequently used keywords.

The most cited paper with almost 250 citations is a tutorial review on the use of multi way techniques and fluorescence spectroscopy. The article refers specifically to parallel factor analysis (PARAFAC) used to decompose tri-linear data sets such as those arising from excitation emission matrices (EEM) of fluorescence applications<sup>48</sup>. Interestingly and despite the suitability of fluorescence technology to evaluate water samples, the keyword fluorescence was not found within the 20 most used keywords. Another paper with a significant number of citations was published in Food and Chemical Toxicology from an international collaboration between Turkey and Saudi Arabia. The article attempts the use of spectrophotometry and more specifically visible measurements at 506 nm to quantify the levels of allura red dye in preconcentrated water samples<sup>69</sup>. A solid phase extraction procedure was optimized and allura red levels can be quantified at µg levels with variation coefficients of 7%<sup>69</sup>. The studies identified here are not always devoted to the evaluation of water samples. Some of the applications are based on quantification of water content whereas other focus on the quantification of analytes dissolved in water and beverages.

Wine. In this case *near* and *mid infrared*, in this order are the techniques of preference to evaluate the *quality* of *grapes* and wines during the *fermentation* process. The use of *reflectance* spectroscopy seems to also be a priority for *grapes* and wine applications. An intense emphasis in quality control of *grape* samples and also monitoring of the *fermentation* progression using spectroscopy applications can be depicted from the keyword analysis. *Phenolic compounds*, probably due to its *antioxidant* properties, is one of the most frequently used keyword and shows the high interest in the quantification of this crucial compounds, analysed mostly with *HPLC* for wine *quality* evaluation. *Classification*, *prediction* and *discrimination* tasks are commonly employed and often used for wine or cultivar *authentication*.

The most cited paper was published in *Food Research International* in 2009 by a group of Spanish researchers. The study makes use of NIR spectroscopy in transmittance mode to

quantify reducing sugar in grapes, fermenting samples and wines<sup>70</sup>. Accurate calibration was for this parameter were reported. The authors also identified 4 key wavelengths, named as fingerprint spectra, that could potentially be used to develop a low cost instrument<sup>70</sup>. The second most prolific paper, published in the same journal and year, evaluated the ability of nuclear magnetic resonance (NMR) spectroscopy coupled with multivariate data analysis to discriminate between wines made with four different cultivars. Principal component analysis (PCA) and orthogonal projection in latent structures discriminant analysis (OPLS-DA) were successfully employed for the discrimination task<sup>71</sup>. The third most prolific article presents a review on the potential use of front face fluorescence spectroscopy as a control tool for the wine industry<sup>72</sup>. This paper was also published by a group of Spanish researchers in Food Research International journal. PARAllel FACtor Analysis (PARAFAC) and fluorescence excitation emission matrices (EEMs) were used to discriminate samples based on appellation and ageing condition. The fluorescence ability of some wine components such as phenolic and carbonyl compounds showed the potential of this technique for winemaking control strategies. Geographical or cultivar discrimination was observed as a recurrent topic. The analysis of wine antioxidants such as phenolic compounds using a variety of spectroscopy approaches was also widely reported. Finally, strong emphasis was placed on the evaluation of grapes and on the analysis during the fermentation process of wines.

#### **Concluding remarks.**

This study shows and overview of the current status of the spectroscopy research field in food science and technology. The evaluation of indicators of scientific productivity made the identification of the most prolific journals possible. The leading journals in this field were also identified through the evaluation of its impact factor and citation counts. The most prolific institutions and countries in terms of productivity and collaboration were targeted through social network analysis. Finally, the keyword analysis provided relevant information and shed light into the techniques, applications, food products and attributes of interest. A further evaluation of the most widely represented food products was also attempted with relevant information being extracted. The increase in the number of publications in the last years shows the relevance of the spectroscopy research field for food science and technology applications. Spectroscopy has proved to be highly suitable for food products. This includes applications for the totality of the food production chain from the growing and farming of

617 food products to manufacturing and packaging and also during postharvest until final  
618 destination to the consumer.

619 In order to maintain food quality standards, the food industry is in need of reliable, robust,  
620 efficient and inexpensive analytical tools. Spectroscopy applications meet all these  
621 requirements and thus appear as ideal candidates. In addition, the multi-parametric nature  
622 (a single spectral measurement can quantify multiple analytes) and the possibility to perform  
623 spectral readings at-line, in-line or on-line, in a non-destructive nature fulfils the requirements  
624 to ensure food quality and safety standards. The development of spectroscopy applications  
625 goes hand by hand with the development of chemometric tools. New advances in the field of  
626 chemometrics are boosting the number and accuracy of the spectroscopy calibrations  
627 reported. The development of linear and most importantly non-linear regression methods,  
628 including machine learning techniques is also promoting the success of new spectroscopy  
629 applications. Novel spectral pre-processing and variable selection algorithms are also  
630 continuously being reported, helping in the identification of the containing fingerprint regions  
631 in the spectrum, including the treatment of three dimensional data from fluorescence  
632 spectra. Improvements in instrumentation, directly related with spectral quality and probes  
633 suitable for different sample formats are also escorting the implementation of these  
634 applications into food production processes. Despite all this progress, new developments in  
635 the form of hand help transportable devices are still required. The miniaturization of  
636 benchtop/laboratory instrumentation is challenging and changes in spectral quality are often  
637 observed in portable instruments for in field or at-line measurements. New developments in  
638 smaller instrumentation is expected to further promote the incorporation of spectroscopy in  
639 food applications.

640 From the results observed it can be concluded that near infrared is the preferred technique  
641 for food analysis, Raman spectroscopy and its surface enhanced approach (SERS), mid  
642 infrared spectroscopy with the use of attenuated total reflectance and fluorescence  
643 spectroscopy were also widely used. Visible spectroscopy, for colour assessment was also  
644 identified, especially for fruit and vegetables applications. Another important observation  
645 was the preference for reflectance spectral measurements. The convenience of these  
646 applications relies on the possibility of non-destructive direct measurements in fruits,  
647 vegetables, cereals or muscular tissue in the case of meat products. Moreover, intense

research activity was identified for olive oil, meat (mainly beef and pork), fruits, specially apples, wheat and cereals and finally water and wine.

Olive oil applications focussed on authentication and adulteration tasks with Raman spectroscopy as the most common used technique. For fruit applications NIR spectroscopy in reflectance mode was widely explored for internal properties evaluation. Moreover, NIR and Raman were observed for prediction, authentication and adulteration exercises of meat with measurements very often taking place on direct muscular tissues. Authentication and adulteration were also key focus areas for milk and dairy product with fluorescence spectroscopy applications being observed. In the case of wine, the focus is placed in grape evaluation using reflectance technology and NIR and MIR applications for fermentation monitoring with a strong focus on phenolic compounds. Wine adulteration was also found as a hot topic.

Concerns raised by researchers in terms of robustness and accuracy of the calibrations are frequently observed in the literature. These emphasise the need of appropriate sample sets containing enough relevant variability to ensure the accuracy of further predictions. The evaluation of model performance over time was also a re-current topic for some applications. Furthermore, the developed spectroscopy applications need to become part of integrated systems that can be implemented in industrial setups. The multi-parametric nature of spectroscopy applications raises the need for integrated systems where the information is condensed and delivered in a simplistic manner. This needs of multivariate process control approaches, including multi-evaluation strategies that will require not only prediction tasks but also classification, identification or discrimination exercises, as has been widely reported in the literature. Moreover, the majority of the studies still make use of benchtop instrumentation or laboratory setups with direct measurements on the sample tissue. Despite not being frequently identified in this study, contactless spectroscopy in reflectance mode is proposed as a major solution for industrial applications.

Development on instrumentation and data analysis are causing the appearance of more and more food applications. Moreover, the body of research and exponential growth observed suggest the gradual incorporation of spectroscopy applications in the everyday food quality control operations. The role of spectroscopy in the food industry is therefore expected to progressively increase in the near future. Finally, future bibliometric studies might confirm

the expected progression of this research topic, the appearance of collaborations between existing and new role players and the consolidation of spectroscopy as the analytical reference technique for the food industry.

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Figure 1 Number of published paper and citations received for the 2009-2018 period

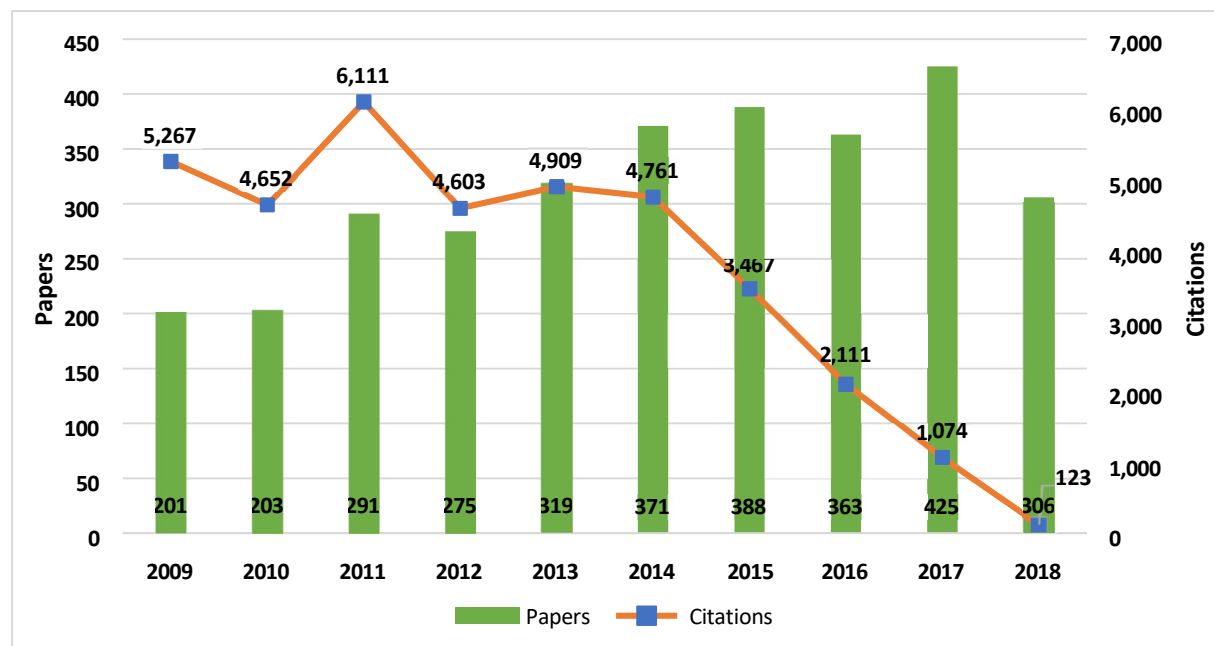




Figure 2 Main network of institutions' collaboration. A threshold of more than two collaborations in common was applied. The size of the spheres indicates the number of collaborations for a particular institution, whereas the thickness of the line indicates to intensity of the collaboration. Bigger spheres or thicker lines indicate higher number of collaborations and more intense collaboration between two institutions

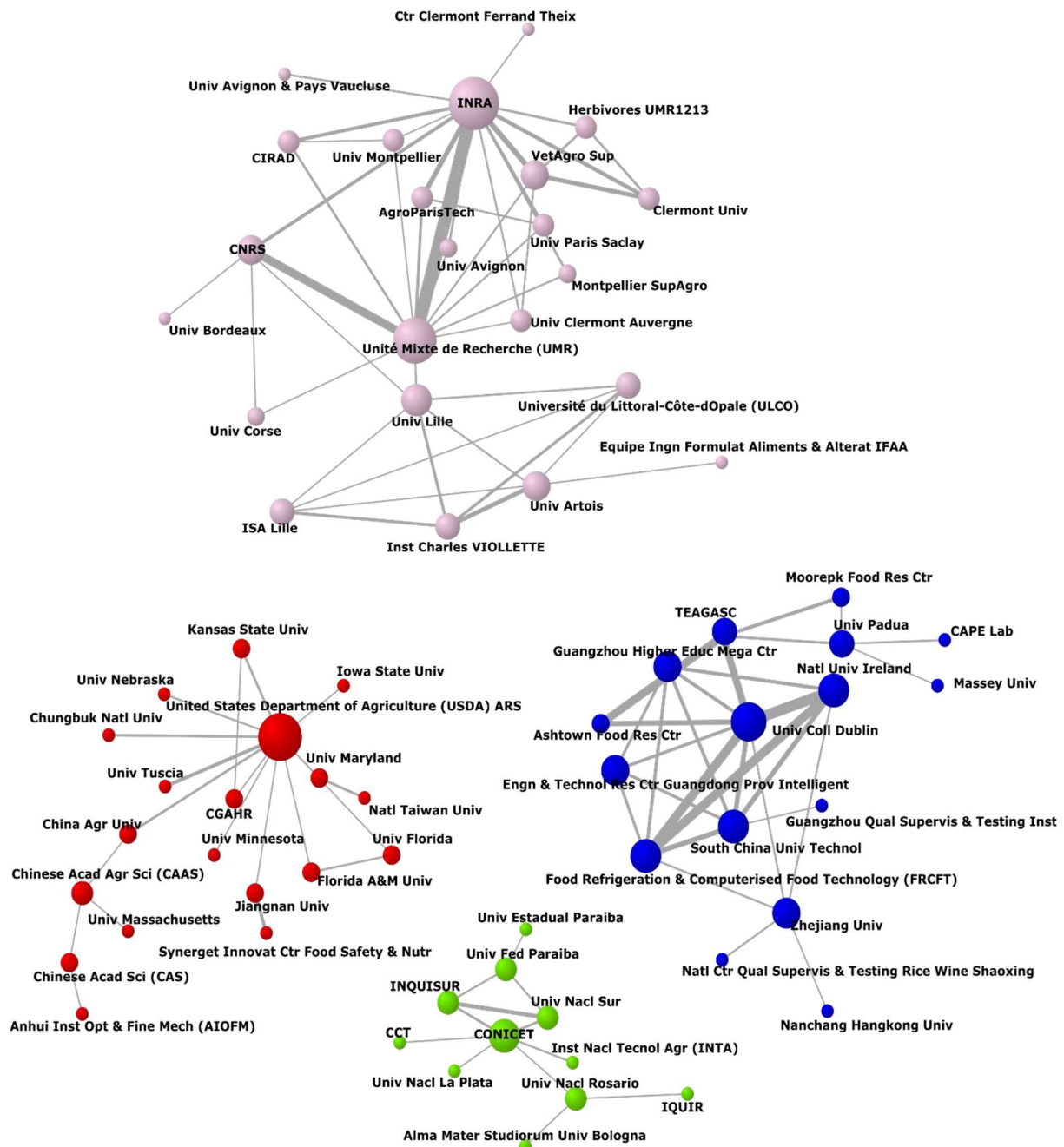


Figure 3 Global scientific production and international collaboration on spectroscopy. The size of the spheres is proportional to the number of publications, whereas the thickness of the line is proportional to the intensity of the collaboration (papers published in collaboration between two countries).



Figure 4 Keyword network for spectroscopy. Seventy-three words with more than forty-five co-occurrences are represented. The size of the spheres represents the number of times the keyword was used, whereas the thickness of the lines indicates the intensity of the co-occurrence. Thicker lines indicate a more frequent appearance of the pair of keywords in a publication.

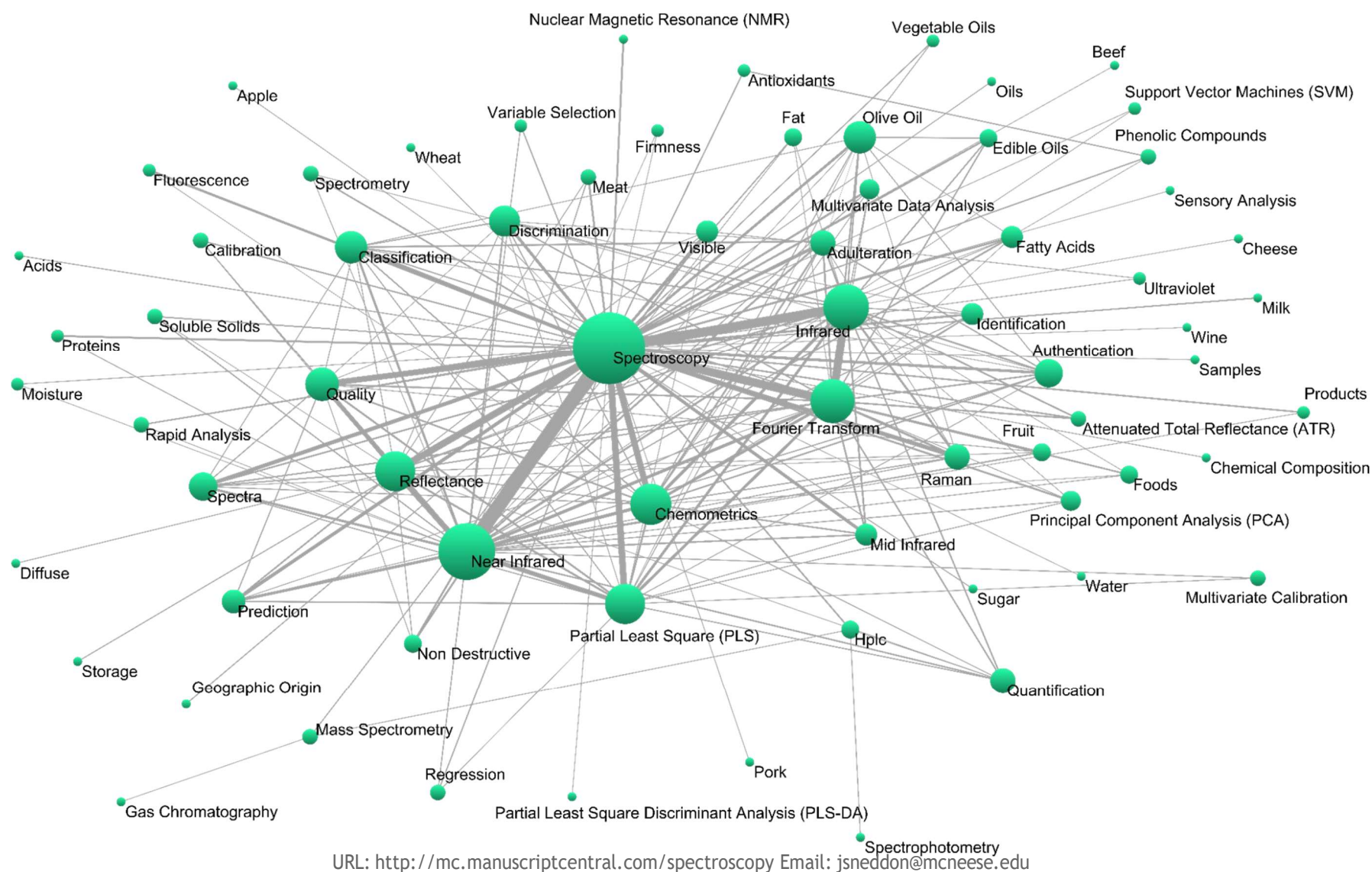


Table 1 Number of papers in most productive journals, citations, citations per article, impact factor, and subject category (journals with more than 40 papers are shown)

Journal	Country	Papers	Citations	Citations/papers	IF 5 years	Web of Science Subject category	Quartile
Food Chemistry	England	458	8,540	18.65	4.946	Chemistry, Applied Food Science & Technology Nutrition & Dietetics	Q1 Q1 Q1
Analytical Methods	England	454	3,300	7.27	2	Chemistry, Analytical Food Science & Technology Spectroscopy	Q3 Q2 Q2
Journal of Agricultural and Food Chemistry	USA	259	5,109	19.73	3.791	Agriculture, Multidisciplinary Chemistry, Applied Food Science & Technology	Q1 Q1 Q1
Food Analytical Methods	USA	197	1,087	5.52	2.2	Food Science & Technology	Q2
Journal of AOAC International	USA	101	402	3.98	1.102	Chemistry, Applied Food Science & Technology	Q4 Q3
Journal of Food Engineering	England	100	1,462	14.62	3.851	Engineering, Chemical Food Science & Technology	Q1 Q1
Food Control	England	86	964	11.21	3.891	Food Science & Technology	Q1
Food Research International	USA	83	1,921	23.14	4.196	Food Science & Technology	Q1
LWT-Food Science and Technology	England	80	929	11.61	3.455	Food Science & Technology	Q1
Meat Science	England	78	1,577	20.22	3.55	Food Science & Technology	Q2
Journal of Dairy Science	USA	73	998	13.67	3.085	Agriculture, Dairy & Animal Science Food Science & Technology	Q1 Q2
International Journal of Food Properties	USA	70	247	3.53	161	Food Science & Technology	Q2
Journal of the Science of Food and Agriculture	England	65	418	6.43	2.537	Chemistry, Applied Food Science & Technology Agriculture, Multidisciplinary	Q2 Q2 Q1
Journal of Food Science	USA	57	643	11.28	2.307	Food Science & Technology	Q2
Food and Bioprocess Technology	USA	56	1,367	24.41	3.325	Food Science & Technology	Q1
Journal of the American Oil Chemists Society	USA	52	558	10.73	1.863	Chemistry, Applied Food Science & Technology	Q3 Q3
Postharvest Biology and Technology	Netherlands	46	721	15.67	3.241	Agronomy Food Science & Technology Horticulture	Q1 Q1 Q1
Journal of Food Composition and Analysis	USA	43	702	16.33	3.224	Chemistry, Applied Food Science & Technology	Q2 Q1

Table 2 Most cited papers (hot papers), authors, journal, citations and standardized citations. A threshold of > 100 papers was applied

Authors	Title	Source	Citations	Standardized citations
Murphy, KR; Stedmon, CA; Graeber, D; Bro, R	Fluorescence spectroscopy and multi-way techniques. PARAFAC	Analytical Methods 2013; 5(23): 6557-6566	246	41.00
Prieto, N; Roehe, R; Lavin, P; Batten, G; Andres, S	Application of near infrared reflectance spectroscopy to predict meat and meat products quality: A review	Meat Science 2009; 83(2): 175-186	217	21.70
Mauer, LJ; Chernyshova, AA; Hiatt, A; Deering, A; Davis, R	Melamine Detection in Infant Formula Powder Using Near- and Mid-Infrared Spectroscopy	Journal of Agricultural and Food Chemistry 2009; 57(10): 3974-3980	187	18.70
Lerma-Garcia, MJ; Ramis-Ramos, G; Herrero-Martinez, JM; Simo-Alfonso, EF	Authentication of extra virgin olive oils by Fourier-transform infrared spectroscopy	Food Chemistry 2010; 118(1): 78-83	177	19.67
Lopez-Moreno, ML; de la Rosa, G; Hernandez-Viezcas, JA; Peralta-Videa, JR; Gardea-Torresdey, JL	X-ray Absorption Spectroscopy (XAS) Corroboration of the Uptake and Storage of CeO2 Nanoparticles and Assessment of Their Differential Toxicity in Four Edible Plant Species	Journal of Agricultural and Food Chemistry 2010; 58(6): 3689-3693	161	17.89
Yuan, TQ; Sun, SN; Xu, F; Sun, RC	Characterization of Lignin Structures and Lignin-Carbohydrate Complex (LCC) Linkages by Quantitative C-13 and 2D HSQC NMR Spectroscopy	Journal of Agricultural and Food Chemistry 2011; 59(19): 10604-10614	156	19.50
Rohman, A; Man, YBC	Fourier transform infrared (FTIR) spectroscopy for analysis of extra virgin olive oil adulterated with palm oil	Food Research International 2010; 43(3): 886-892	155	17.22
Gomez-Ordonez, E; Ruperez, P	FTIR-ATR spectroscopy as a tool for polysaccharide identification in edible brown and red seaweeds	Food Hydrocolloids 2011; 25(6): 1514-1520	148	18.50
Craig, AP; Franca, AS; Irudayaraj, J	Surface-Enhanced Raman Spectroscopy Applied to Food Safety	Annual Review of Food Science and Technology 2013; 4(): 369-380	132	22.00
Magwaza, LS; Opara, UL; Nieuwoudt, H; Cronje, PJR; Saeys, W; Nicolai, B	NIR Spectroscopy Applications for Internal and External Quality Analysis of Citrus Fruit-A Review	Food and Bioprocess Technology 2012; 5(2): 425-444	124	17.71
Randviir, EP; Banks, CE	Electrochemical impedance spectroscopy: an overview of bioanalytical applications	Analytical Methods 2013; 5(5): 1098-1115	122	20.33
Pereira, L; Amado, AM; Critchley, AT; van de Velde, F; Ribeiro-Claro, PJA	Identification of selected seaweed polysaccharides (phycocolloids) by vibrational spectroscopy (FTIR-ATR and FT-Raman)	Food Hydrocolloids 2009; 23(7): 1903-1909	120	12.00
Seruga, M; Novak, I; Jakobek, L	Determination of polyphenols content and antioxidant activity of some red wines by differential pulse voltammetry, HPLC and spectrophotometric methods	Food Chemistry 2011; 124(3): 1208-1216	114	14.25
Pan, XR; Qin, PF; Liu, RT; Wang, J	Characterizing the Interaction between Tartrazine and Two Serum Albumins by a Hybrid Spectroscopic Approach	Journal of Agricultural and Food Chemistry 2011; 59(12): 6650-6656	112	14.00
Yuen, SN; Choi, SM; Phillips, DL; Ma, CY	Raman and FTIR spectroscopic study of carboxymethylated non-starch polysaccharides	Food Chemistry 2009; 114(3): 1091-1098	108	10.80



Mangolim, CS; Moriwaki, C; Nogueira, AC; Sato, F; Baesso, ML; Neto, AM; Matioli, G	Curcumin-beta-cyclodextrin inclusion complex: Stability, solubility, characterisation by FT-IR, FT-Raman, X-ray diffraction and photoacoustic spectroscopy, and food application	Food Chemistry 2014; 153(): 361-370	105	21.00
Maggio, RM; Kaufman, TS; Del Carlo, M; Cerretani, L; Bendini, A; Cichelli, A; Compagnone, D	Monitoring of fatty acid composition in virgin olive oil by Fourier transformed infrared spectroscopy coupled with partial least squares	Food Chemistry 2009; 114(4): 1549-1554	104	10.40
Lachenmeier, DW; Humpfer, E; Fang, F; Schutz, B; Dvorsak, P; Sproll, C; Spraul, M	NMR-Spectroscopy for Nontargeted Screening and Simultaneous Quantification of Health-Relevant Compounds in Foods: The Example of Melamine	Journal of Agricultural and Food Chemistry 2009; 57(16): 7194-7199	104	10.40
Chi, ZX; Liu, RT; Teng, Y; Fang, XY; Gao, CZ	Binding of Oxytetracycline to Bovine Serum Albumin: Spectroscopic and Molecular Modeling Investigations	Journal of Agricultural and Food Chemistry 2010; 58(18): 10262-10269	103	11.44
Bobelyn, E; Serban, AS; Nicu, M; Lammertyn, J; Nicolai, BM; Saeys, W	Postharvest quality of apple predicted by NIR-spectroscopy: Study of the effect of biological variability on spectra and model performance	Postharvest Biology and Technology 2010; 55(3): 133-143	103	11.44

Table 3 Most frequently used keywords for the combination of the different food product and spectroscopy. The number of co-occurrences between spectroscopy and the food product is indicated in brackets.

	Olive oil(163)	Apple(52)	Beef(48)	Cheese(47)	Fruit(107)	Meat(123)	Milk(86)	Pork(50)	Water(46)	Wheat(48)	Wine(47)
1	Fourier Transform	Near Infrared	Meat	Near Infrared	Near Infrared	Near Infrared	Near Infrared	Near Infrared	Food	Near Infrared	Near Infrared
2	Infrared	Reflectance	Reflectance	Infrared	Quality	Reflectance	Infrared	Meat	Near Infrared	Quality	Partial Least Square (PLS)
3	Adulteration	Fruit	Near Infrared	Milk	Reflectance	Quality	Chemometrics	Reflectance	HPLC	Reflectance	Classification
4	Edible Oils	Non Destructive	Quality	Chemometrics	Non Destructive	Infrared	Adulteration	Quality	Preconcentration	Fourier Transform	Phenolic Compounds
5	Chemometrics	Quality	Chemometrics	Fluorescence	Soluble Solids	Pork	Fourier Transform	Water Holding Capacity	Spectrophotometry	Infrared	Infrared
6	Authentication	Firmness	Infrared	Fourier Transform	Apple	Beef	Fluorescence	Infrared	Atomic Emission Spectrometry	Grain	Chemometrics
7	Vegetable Oils	Soluble Solids	Pork	Geographic Origin	Partial Least Square (PLS)	Raman	HPLC	Prediction	Cloud Point Extraction	Partial Least Square (PLS)	Fourier Transform
8	Classification	Visible	Spectra	Mid Infrared	Prediction	Chemometrics	Mid Infrared	Partial Least Square (PLS)	Infrared	Proteins	Mid Infrared
9	Raman	Prediction	Partial Least Square (PLS)	Quality	Firmness	Partial Least Square (PLS)	Partial Least Square (PLS)	Beef	Partial Least Square (PLS)	Chemometrics	Food
10	Near Infrared	Internal Quality	Fatty Acids	Spectra	Food	Prediction	Cheese	Colour Fourier Transform	Quality	Spectra	Prediction
11	Fatty Acids	Partial Least Square (PLS)	Muscle	Partial Least Square (PLS)	Antioxidants	Classification	Food Quantification	Spectra	Chromatography	Barley	Data Analysis
12	Partial Least Square (PLS)	Soluble Solids Content	Raman	Proteins	Fourier Transform	Fourier Transform				Nuclear Magnetic Resonance (NMR)	Fermentation
13	Quality	Storage	Colour	HPLC	vegetables	Spectra	Dairy Products	Muscle	Nuclear Magnetic Resonance (NMR)		
14	Nuclear Magnetic (NMR)			Nuclear Magnetic (NMR)				Early Post Mortem	Spectrometry	Products	Spectra
15	Spectra	Sugar	Fluorescence	Authentication	Infrared	Adulteration	Quality	Chemometrics	Moisture	Raman	Grapes
16	Food	Diffuse	Tenderness	Fatty Acids	Sugar	Discrimination	Reflectance	Classification	Extraction	Transmittance	Quality
17	Discrimination	Infrared	Adulteration	Dairy Products	Visible	Authentication	Tandem Mass Spectrometry	Fatty Acids	Fourier Transform	Fluorescence	HPLC
18	Fluorescence	Calibration	Food	Discrimination	Storage Phenolic Compounds	Identification	Fat	Products	Meat	Moisture	Reflectance
19	Mid Infrared	Dry Matter	Quantification	Food		Water Holding Capacity	Authentication	Raman	Quantification	Plants	Antioxidants
20	Phenolic Compounds	Fourier Transform	Chemical Composition	Products	HPLC	Chemical Composition	Raman	Sensory Analysis	Spectra	Starch	Authentication

Table 4 Most cited papers for the different identified food products with authors, journal and citation counts

Olive oil			
Authors	Title	Journal	Citations
Lerma-Garcia, M. J.; Ramis-Ramos, G.; Herrero-Martinez, J. M.; Simo-Alfonso, E. F.	Authentication of extra virgin olive oils by Fourier-transform infrared spectroscopy	Food Chemistry 2010; 118(1): 78-83	177
Rohman, A.; Man, Y. B. Che	Fourier transform infrared (FTIR) spectroscopy for analysis of extra virgin olive oil adulterated with palm oil	Food Research International 2010; 43(3): 886-892	155
Maggio, Ruben M.; Kaufman, Teodoro S.; Del Carlo, Michele; et al.	Monitoring of fatty acid composition in virgin olive oil by Fourier transformed infrared spectroscopy coupled with partial least squares	Food Chemistry 2009; 114(4): 1549-1554	104
Sinelli, Nicoletta; Cerretani, Lorenzo; Di Egidio, Valentina; Bendini, Alessandra; Casiraghi, Ernestina	Application of near (NIR) infrared and mid (MIR) infrared spectroscopy as a rapid tool to classify extra virgin olive oil on the basis of fruity attribute intensity	Food Research International 2010; 43(1): 369-375	87
Karoui, Romdhane; Blecker, Christophe	Fluorescence Spectroscopy Measurement for Quality Assessment of Food Systems-a Review	Food and Bioprocess Technology 2011; 4(3): 364-386	78
Lohumi, Santosh; Lee, Sangdae; Lee, Hoonsoo; Cho, Byoung-Kwan	A review of vibrational spectroscopic techniques for the detection of food authenticity and adulteration	Trends in Food Science & Technology 2015; 46(1): 85-98	64
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