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### ► To cite this version:

Weijie Lan, Benoit Jaillais, Catherine M.G.C. Renard, Alexandre Leca, Songchao Chen, et al.. A method using near infrared hyperspectral imaging to highlight the internal quality of apple fruit slices. *Postharvest Biology and Technology*, 2021, 175 (1), pp.111497. 10.1016/j.postharvbio.2021.111497 . hal-03182741

**HAL Id: hal-03182741**

**<https://hal.inrae.fr/hal-03182741>**

Submitted on 13 Feb 2023

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1 **A method using near infrared hyperspectral imaging to highlight the internal**  
2 **quality of apple fruit slices**

3

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29 **Highlights**

30 Near-infrared hyperspectral imaging assessed the apple heterogeneity.

31 Principal component analysis allowed to select the region of interest in apples.

32 Single apple presented a large heterogeneity of biochemical compositions.

33 Models mapped total sugars and dry matter contents in each apple.

34

35 **Abstract**

36 The heterogeneity of apple fruit was highlighted by near-infrared hyperspectral  
37 imaging (NIR-HSI) using a data analysis in two successive steps. First, NIR-HSI  
38 images were acquired on the cut surface of six transverse slices per apple, which were  
39 then systematically sampled with 5 or 6 cylinders per slice. PCA carried out on the  
40 NIR-HSI images allowed to select 141 representative cylinders from the total dataset  
41 (1056 samples), in which the contents of dry matter (DMC), total sugars (TSC),  
42 fructose, glucose, sucrose, malic acid and polyphenols were quantified by  
43 spectrophotometry and chromatography. In a second step, leave-one-out PLS models  
44 were developed and successfully used to describe the distribution of DMC ( $R_{cv}^2 =$   
45 0.83, RPD = 2.39) and TSC ( $R_{cv}^2 = 0.81$ , RPD =2.20) in each apple slice. A strong  
46 heterogeneity of DMC and TSC was detected inside each fruit. Such a simple and  
47 rapid method reduced the needs of numerous chemical characterizations to  
48 demonstrate the distribution of quality traits within and between fruit and contributed  
49 to better manage the fruit quality measurements.

50 **Keywords:** *Malus domestica* Borkh.; partial least square regression; random forest  
51 regression; apple variability and heterogeneity.

52

## 53 **Introduction**

54 An external aesthetic appearance and a sustainable internal quality of fruit are  
55 both crucial for consumers (Ma et al., 2018; Zhang et al., 2018). However, genetic  
56 diversity (varieties), pedoclimatic conditions and agricultural practices are known to  
57 provide variability and heterogeneity of fruit, which limit the precision and prediction  
58 of quality using infrared methods (Vis-NIR and NIRS) and thus hinders their  
59 widespread applications for online commercial fruit sorting (Barritt et al., 1991; Xia et  
60 al., 2020; Zhang et al., 2018). It appears necessary to develop some applications using  
61 efficient and rapid technologies to phenotype internal heterogeneity of the fruit, in  
62 order to help field growers and industrial manufacturers to improve quality of fruit  
63 products.

64 Apple is one of the most consumed agricultural commodities in the global fruit  
65 market (68.6 million tons at 2018) (USDA, 2018). The high heterogeneity of soluble  
66 solids content (Fan et al., 2016; Mo et al., 2017; Peiris et al., 1999), starch (Menesatti  
67 et al., 2009), polyphenols and vitamin C (Pissard et al., 2012) in a single apple fruit  
68 has been proven to truly exist in different directions, from proximal to distal direction  
69 (Fan et al., 2016; Peiris et al., 1999), in radial direction from inside to outside (Mo et  
70 al., 2017) and along equatorial direction (Mo et al., 2017; Pissard et al., 2012).

71 As known, conventional chemical analyses (HPLC-DAD, GC-MS and  
72 ultraviolet/ visible spectrometry etc.) are costly and time-consuming to determine the  
73 heterogeneity occurring at the level of the tissues in a single fruit (Peng et al., 2019;  
74 Pissard et al., 2012). To determine the chemical heterogeneity within a fruit, most

75 previous works encountered difficulties of i) long-periods and intensive labor  
76 operations, ii) a large amount of targeted fruit samples and the high requirements for  
77 characterization, and iii) the limited stability of fruit samples (highly hydrated, rapid  
78 oxidation). In addition, the limited knowledge of apple heterogeneity becomes a  
79 barrier to obtain robust predictive models by high-throughput techniques (Vis-NIRS,  
80 NIRS, MIRS, NMR) (de Oliveira et al., 2014; Fan et al., 2016; Pissard et al., 2012).  
81 Particularly with the non-destructive and localized (around 2 cm<sup>2</sup>) NIR measurements  
82 on apples, it is essential to know more about the distribution of components in fruit in  
83 order to determine where and how many measurements are needed, as well as to  
84 access the representative sample portion to be characterized using reference methods  
85 for calibration dataset.

86       Hyperspectral imaging (HSI) is an emerging platform technique that integrates  
87 imaging and spectroscopy to provide both spatial and spectral information (Gowen et  
88 al., 2007). It is safer than X-ray imaging, more rapid and affordable than FT-IR  
89 imaging and Magnetic resonance imaging, and with a better image quality than  
90 thermal imaging (Fan et al., 2016; Ma et al., 2018). Until now, applications of HSI in  
91 the Visible-NIR (400-1000 nm) or NIR (1000-2400 nm) ranges were carried out to  
92 evaluate the variability of apple quality, such as fruit defects (Mehl et al., 2004),  
93 firmness (Peng and Lu, 2008), mealiness (Huang and Lu, 2010) and soluble solids  
94 content (Mendoza et al., 2011). These studies were applied nondestructively on apple  
95 fruit. As the NIRS radiation penetration depth is around 0.2 to 0.3 cm in the spectral  
96 area between 900 and 1900 nm (Lammertyn et al., 2000), the non-destructive

97 detection of HSI does not allow to evaluate the entire internal heterogeneity of apple  
98 fruit. Thus, the HSI is used destructively by scanning fruit slices and makes possible  
99 to describe the distribution of the internal soluble solids content, as shown in apples  
100 (Mo et al., 2017) and melons (Sun et al., 2017). However, these studies need a large  
101 number of reference data (numbers of samples and limited samples quantity) on all  
102 the targeted areas of single fruit, required for model calibration.

103 Consequently, the main objective of this work was to provide a simple and  
104 efficient method to reduce the intensive reference measurements (contents of dry  
105 matter, total sugars, individual sugars, acids and polyphenols) in order to develop a  
106 HSI modelling calibration and to evaluate the apple variability and heterogeneity.

## 107 **2. Material and methods**

### 108 2.1 Apple fruit

109 The experiment was conducted on four different apple varieties: ‘Golden  
110 Delicious’ (GD), ‘Granny Smith’ (GS), ‘Braeburn’ (BR) and ‘Royal Gala’ (GA). In  
111 2018, all apples were harvested in the experimental orchard at La Pugère (Bouches du  
112 Rhône, France). ‘Braeburn’, ‘Granny Smith’ and ‘Royal Gala’ apples were grown  
113 under a commercial fruit thinning (Th+, 50-100 fruit/ tree). ‘Golden Delicious’ apples  
114 were grown under two thinning conditions, the commercial fruit thinning (Th+,  
115 50-100 fruit/ tree) and without thinning (Th-, 150-200 fruit/ tree). After the  
116 commercial harvesting (‘Royal Gala’ on August 28<sup>th</sup>, Golden Delicious on September  
117 19<sup>th</sup>, ‘Granny Smith’ on September 20<sup>th</sup>, and ‘Braeburn’ on October 3<sup>rd</sup>), all apples  
118 were stored in a cold chamber at 4 °C and at around 90 % of humidity until their

119 characterization (November 2018).

## 120 2.2 Samples preparation

121 A calibration dataset corresponded to the data of 30 apples with similar sizes (6  
122 fruit  $\times$  5 apple groups of GD Th-,GD Th+, GS, BR, GA) and scanned using the  
123 NIR-HSI imaging system. Each apple was cut with a slicing tool along horizontal  
124 direction to produce six apple slices, including five 1.2 cm thick slices (named slices  
125 from 'A' to 'E' at the stem, equator and calyx directions) and the one residual piece of  
126 varying thickness (named slice 'F' at the calyx positions). Hyperspectral images of  
127 180 apple slices (5 apple groups  $\times$  6 fruit  $\times$  6 slices) were acquired and six cylindrical  
128 1.6 cm diameter portions were extracted with a cookie cutter (numbered 1 to 6) from  
129 each of the apple slices A to E, and five or six cylinders from the residual slice F (**Fig.**  
130 **1**).

131 The cylinders were put immediately in liquid nitrogen prior to storage at -20 °C,  
132 giving 35 to 36 cylinders per apple, following the previous works of Mo et al. (2017)  
133 and Bureau et al. (2013). These cylinders were distributed with a systematic  
134 repartition for each apple from the top to the bottom and from the sunny to the shady  
135 faces. In total 1056 cylinders (5 apple groups  $\times$  6 fruit  $\times$  35-36 cylinders) were  
136 numbered and stored (**Part 2.4.1**). After the extraction of all the cylinders, RGB  
137 photos were taken on each apple slice in order to ensure the correct correspondence  
138 between the cylinders and HSI images (**Fig. 1**).

## 139 2.3 Hyperspectral Imaging (HSI) System

140 A pushbroom (a line-scanning type) near infrared hyperspectral imaging system



141 (SPECIM, Oulu, Finland) was used to acquire the hyperspectral images of apple slices.  
142 Particularly, this NIR-HSI system consisted of a SWIR camera (SWIR-CL-400-N25E,  
143 SPECIM) covering the spectral range of 1000-2500 nm with a spectral resolution of  
144 about 12 nm, an OLES 56 camera lens (SPECIM), an illumination source (halogen  
145 lamps) and a translating scanner. All the image acquisition parameters (the exposure  
146 time of camera, the scanning speed etc.) were controlled by the LUMO® software  
147 from SPECIM. Before measurements, a reflectance calibration was performed by  
148 recording a dark current image (0 % reflectance) with an internal shutter and a white  
149 image using a reference standard close to 100 % reflectance (Spectralon® 100 %). To  
150 reduce the impact of light and noise, the calibrated hyperspectral images could be  
151 automatically obtained using the dark and white reference images, with the following  
152 equation:

$$153 \quad R(\lambda) = \frac{R_0(\lambda) - R_d}{R_w - R_d} \times 100 \% \quad (1)$$

154 with  $R$ : the calibrated hyperspectral image data,  $R_0$ : the raw image data,  $R_d$  and  $R_w$ :  
155 the dark and white reference images, respectively.

156 All images were acquired in the reflectance mode and the final image size for  
157 each kernel is  $387 \times \text{xdim} \times 288$ , the two first values representing pixel dimensions in  
158 the x and y directions (field of view of  $9.8 \times 6.3$  cm, with a spatial resolution of 225  
159  $\mu\text{m}$ ) and the third value accounting for the number of spectral channels. The xdim  
160 values varied according to the dimensions of apple slices. Each image was acquired in  
161 about twenty seconds. As the beginning and ending wavelengths contained noise  
162 caused by the instrument itself (Sun et al., 2017), the 258 bands from 990 to 2450 nm

163 were selected for further spectral analysis.

#### 164 2.4 Imaging pre-processing

165 The pre-processing of the hyperspectral images and the selection of region of  
166 interest (ROIs) were performed with Matlab 7.5 (Mathworks Inc. Natick, MA)  
167 software using the SAISIR package (Cordella & Bertrand, 2014). Due to the high  
168 volume of data, the processing of all images was not possible using a common  
169 computer. In this way, 10,000 spectra were randomly extracted from the HSI images  
170 of each apple slice, counting around one third of the total number of spectra in each  
171 HSI image. Afterwards, all random selected spectra were gathered into a matrix  $X$  (5  
172 apple groups  $\times$  6 fruit  $\times$  6 slices  $\times$  10,000 rows by 258 columns). After pre-tests,  
173 matrix  $X$  was smoothed by a window size of three pixels. A given value  $x(i)$  of index  $i$   
174 was replaced by the local average of  $x(i-1) + x(i) + x(i+1)$ . Then it was  
175 pre-processed with standard normal variate (SNV) to increase its signal to noise ratio  
176 for the selection of ROIs.

#### 177 2.5 ROI selection and characterization

178 PCA has been commonly applied on the NIR-HSI of agro-food products for  
179 safety and quality assessments (Dale, et al., 2013). It was performed on the  
180 pre-processed matrix  $X$  to check the major components causing variability in the  
181 apples. Afterwards, this model was applied to all pixels of all images, and the major  
182 components (PCs) were selected as estimators to refold into PCs images to point out  
183 the heterogeneous areas in each HSI image of apple slice. Finally, the ROIs to be  
184 analyzed by chemical and biochemical measurements (141 samples) were manually

185 selected depending on the results of the major principal components and the same  
186 location on photographic images (an example of the ROIs marked black circles in  
187 **Fig. 1**).

## 188 2.6 Chemical and biochemical measurements

189 All chemical and biochemical characterizations (contents of dry matter, fructose,  
190 glucose, sucrose, malic acid and sum of polyphenols) were performed on these ROIs  
191 (141 samples) and expressed as the ratio on fresh weight. Particularly, individual  
192 sugars (glucose, fructose, and sucrose) and malic acid were quantified on the half of  
193 each sample using an enzymatic method with commercial kits for food analysis,  
194 following the manufacturer's instructions (R-biopharm, Darmstadt, Germany). The  
195 total sugars content were computed by the sum of all individual sugars (fructose,  
196 glucose and sucrose). The dry matter content (DMC) was estimated from the weight  
197 of freeze-dried samples upon reaching a constant weight (freeze-drier, 3 days). The  
198 freeze-dried samples were further used to quantify polyphenols by HPLC-DAD after  
199 thioacidolysis as described in Le Bourvellec ([Le Bourvellec et al., 2011](#)). Particularly,  
200 apple polyphenols were separated in an Agilent 1050 separation system coupled with  
201 a (250 mm × 4 mm i.d.) Licrospher PR-18 5 µm column (Merck, Darmstadt,  
202 Germany) operated at 30 °C. This data was presented as the sum of individual  
203 polyphenols including procyanidins and monomeric flavanols, phenolic acids,  
204 dihydrochalcones and flavonols.

## 205 2.7 Modelling

206 After smoothing with a 3-point window and the first order derivative with a 11

207 point window, the averaged spectra of each ROI (giving 141 spectra) and their related  
208 reference data were used for modelling. Leave-one-out partial least squares  
209 (LOO-PLS) regression was used to build prediction models with Matlab 7.5  
210 (Mathworks Inc. Natick, MA) software using the SAISIR package (Cordella &  
211 Bertrand, 2014). Random forest (RF) regression was also applied to compare the  
212 prediction ability of developed models, using R software (version 4.0.2) (R Core  
213 Team, 2019) coupled with several packages including ‘prospectr’ (Stevens and  
214 Ramirez-Lopez, 2014), ‘Rmatlab’ (Bengtsson et al., 2018), ‘caret’ (Kuhn, 2015) and  
215 ‘randomForest’ (Liaw and Wiener, 2002).

216 The developed model performance was assessed using the determination  
217 coefficient of cross-validation ( $R_{cv}^2$ ), the root mean square error of cross-validation  
218 ( $RMSE_{cv}$ ), the number of latent variables (LVs), the ratio of the standard deviation  
219 values (RPD). The interpretations of beta-coefficients were used to determine the  
220 relevant spectral regions. The spectral bands related to the maximum and minimum of  
221 beta-coefficient values can present the most important wavelengths (Sun et al., 2017).

## 222 2.8 Prediction maps of apple quality attributes

223 After comparison of the modeling results of each apple quality attribute, only the  
224 models with RPD values higher than 2.0 allowing a coarse quantitative prediction  
225 (Nicolai et al., 2007), were selected to predict fruit quality attributes of all apple slices  
226 at the individual pixel level. The prediction values were then visualized under the  
227 form of prediction maps, which were used to phenotype the internal distributions of  
228 the predicted quality attributes in apples.

## 229 **3 Results and discussion**

### 230 **3.1 Spectral characteristics**

231 The initial PCA conducted on the random selected spectra of one out of three  
232 pixels of all apple slices (matrix  $X$ ) was able to discriminate the variability and  
233 heterogeneity of apple fruit between the top (slice A) and the bottom (slice F). The  
234 first two principal components represented 68.0 % of the total variability, with the  
235 first component (PC1) of 43.7 % and the second component (PC2) of 24.2 %,   
236 respectively. For all apple groups, a clear discrimination was shown along the first  
237 two principal components (PC1 and PC2) between the middle slices (slices C, D) and  
238 the others (top slices A, B and bottom slices E, F). The most contributing wavelengths  
239 of PC1 and PC2 were: i) the sharp peak around 1065 nm corresponding to the C-H  
240 and O-H stretching in second overtone, which is linked to the sugar variations in fruit  
241 (Sun et al., 2017); ii) the absorption region from 1157 - 1364 nm which is associated  
242 with the first overtone of O-H band in water (Ignat et al., 2014); and iii) the broad  
243 band at 1400-1530 nm which corresponds to the combination of second overtone of  
244 C-H stretching and the first overtone of O-H stretching, already used to determine the  
245 soluble solids content in apples (Zhang et al., 2019). These fingerprint wavelengths  
246 pointed out the variations of water and carbohydrate contents in a single apple, which  
247 were consistent with previous results using chemical measurements (Peiris et al., 1999;  
248 Pissard et al., 2012).

249 In a second step, the variability expressed on the dominant PC1 components  
250 (43.7 % of total variability) was used for phenotyping all apple slices based on a

251 correspondence between the different areas described by a color range, according to  
252 their hyperspectral spectra. PC1 scores-images have directly pointed out the most  
253 variable locations with the color range (**Fig. 1**). ROIs in each apple were targeted at  
254 top slice A, middle slice C and bottom slice E, with the most different colored areas  
255 (such as the area No. 3 of slice C and the area No. 3 of slice F in **Fig. 1**). Besides, the  
256 clear color differences inside the middle slices (area No. 2 and No. 5 of slice D in **Fig.**  
257 **1**) were also selected, depending on apple cultivars. A total of 141 ROIs was manually  
258 selected and characterized by reference chemical measurements to check if these  
259 targeted positions really showed variations consistent with the corresponding  
260 hyperspectral images, and to identify the chemical components responsible for the  
261 heterogeneity observed in PC1 scores images.

### 262 **3.2 Chemical characteristics of ROIs**

263 The boxplot of chemical reference data (**Fig. 2**) of the 141 selected ROIs showed  
264 a large variation of contents of dry matter, total sugars, malic acid and polyphenols in  
265 the different apple cultivars.

266 Royal Gala apples had the most intensive variations of DMC among the five  
267 apple groups (**Fig. 2a**). Conversely, the lowest variations of DMC and of TSC (**Fig.**  
268 **2b**) were observed in the thinned (GD Th+) and non-thinned Golden Delicious (GD  
269 Th-), presenting a relatively limited heterogeneity of DMC and TSC in single GD  
270 apples. The fructose content of Granny Smith (GS) had the lowest variations among  
271 the four cultivars (**Fig. 2c**). Moreover, the contents of polyphenols varied a lot in each  
272 apple cultivar (**Fig. 2f**). Golden Delicious (thinned and non-thinned) ( $0.34 \pm 0.14$  g/kg

273 in non-thinned GD and  $0.34 \pm 0.12$  g/kg in thinned GD) and Royal Gala (GA) ( $0.27 \pm$   
274  $0.14$  g/kg) apples presented a large polyphenolic variation compared to GS apples  
275 ( $0.55 \pm 0.14$  g/kg). This result was different from a previous work showing a small  
276 internal heterogeneity of polyphenols in Gala (Vidot et al., 2019). This inconsistent  
277 result could be due to the difference in the measured targeted areas in apples, only  
278 parts close to the fruit surface (Vidot et al., 2019) versus parts distributed everywhere  
279 inside the entire fruit (our experiment).

280 Concerning the effect of agricultural practices on Golden apple quality, the  
281 average contents of total sugars and malic acid were higher in the thinning condition  
282 (GD Th+) than in the non-thinning one (GD Th-), which was in line with our previous  
283 results observed during the 2017 harvested season (Lan et al., 2020). Interestingly, the  
284 tree thinning treatment, by increasing the individual apple growth potential, led to a  
285 lower variability of malic acid (**Fig. 2f**) and sucrose (**Fig. 2d**) contents in Golden  
286 Delicious apples, with the standard derivation values decreasing from 0.89 to 0.62  
287 g/kg and from 10.9 to 9.3 g/kg, respectively.

288 Consequently, the most variable regions chosen according to the PC  
289 scores-images truly exhibited a large heterogeneity, in agreement with the variations  
290 of the reference values of total sugars, dry matter, malic acid and polyphenols. The  
291 apple internal heterogeneity should be then considered as an important factor for  
292 apple fruit quality characterization and understanding.

### 293 **3.3 Prediction of apple quality traits based on averaged spectra of ROIs**

294 The chemical composition data obtained on the 141 selected ROIs was used to

295 build prediction models validated within this selected subset, using the averaged  
296 spectra of each ROI. Acceptable predictions of DMC (SD = 21.9 mg/g,  $R_{cv}^2 = 0.83$ ,  
297  $RMSE_{cv} = 9.7$  mg/g, RPD = 2.39) and TSC (SD = 18.7 g/kg,  $R_{cv}^2 = 0.81$ ,  $RMSE_{cv} =$   
298 8.4 g/kg, RPD = 2.20) were obtained by LOO-PLS, respectively (**Table 1**). According  
299 to Nicolai et al. (2007), a RPD over 2 indicates the possibility to a coarse qualitative  
300 prediction of the internal attributes of fruit. The linear models (PLS) were much better  
301 than the random forest (RF) (**Table1**), as described by Sun et al. (2017) to predict  
302 soluble solids content in melon fruit. The small number of latent variables (LVs)  
303 employed in PLS models indicated the robust prediction of DMC (LVs = 7) and TSC  
304 (LVs = 5), based on data including different apple varieties and growing agricultural  
305 practices. All predicted DMC and TSC on 141 ROIs by LOO-PLS regression were  
306 well correlated to the measured values, according to their linearity correlation plots  
307 (**Fig. 3a and 3b**). Moreover, the beta-coefficients showed strong positive or negative  
308 bands (**Fig. 3c and 3d**) for both, the PLS regressions of DMC and TSC, including  
309 informative spectral regions at around 1123 nm, 1208 nm, 1389- 1401 nm, 1474-  
310 1480 nm, 1857- 1863 nm and 2319- 2336 nm, which have been widely reported to  
311 estimate water and sugar contents in apple fruit (Giovannelli et al., 2014; Lan et al.,  
312 2020; Peirs et al., 2003). Particularly, six sharp peaks at 1208 nm, 1123 nm, 1389 nm,  
313 1474 nm, 1857 and 2336 nm were identified as being important wavelengths to  
314 predict dry matter content in apples. And the specific wavelengths at 1123 nm, 1401  
315 nm, 1480 nm, 1863 nm and 2319 nm contributed to the determination of total sugars  
316 in apple tissues.



317 However, modelling using the averaged spectra of ROIs showed a limited ability  
318 to predict the individual sugars (fructose, glucose and sucrose), malic acid and sum of  
319 polyphenols (**Table 1**). This was expected and in agreement with the previous work  
320 (Walsh et al., 2020). That could be due to i) their respective lower content in apple  
321 tissues compared with DMC and TSC and ii) the limited chemical variations in our  
322 studied apple varieties. Concerning polyphenols, a larger variation is observed in the  
323 cider apple varieties from 1 to 7 g/kg in apple parenchyma (Sanoner et al., 1999) than  
324 in the dessert varieties, such as those of this study, from 0.6 to 0.9 g/kg (Guyot et al.,  
325 2002) because of their highest content in procyanidins, the main polyphenols. Thus, a  
326 better prediction of these compounds might be obtained taking into account the entire  
327 variability within apple varieties.

328 As mentioned in **section 3.1**, the fingerprint wavelengths of apple variability and  
329 heterogeneity were mainly related to water and carbohydrates. Thus, for these five  
330 apple groups (BR, GA, GS, thinned and non-thinned GD), prediction models based on  
331 the averaged HSI spectra of ROIs and their reference values were suitable to estimate  
332 intensive variations of water and the dominated soluble contents in apple fruit, such as  
333 dry matter and total sugars, but not of individual compounds (fructose, glucose,  
334 sucrose and malic acid) or microcomponents (sum of polyphenols).

### 335 **3.4 Phenotyping apple heterogeneity by HSI**

336 For a more in-depth assessment of the internal composition of each apple, the  
337 best PLS models described in the **Part 3.2** were applied to predict the quality traits at  
338 each pixel on all hyperspectral images of apple slices. The resulting images were

339 presented as ‘prediction maps’ for TSC (**Fig. 4**) for each apple slice. In total, 10 colors  
340 were used to fit the different intervals of the predicted values and pixels with the  
341 similar predicted values appeared in the same color. The prediction results  
342 demonstrated a large variability and heterogeneity of total sugars and dry matter  
343 contents i) in different apple varieties; ii) between individual apple fruit and iii) inside  
344 single fruit.

345 For the traditional non-destructive NIR analyses on apples, to obtain a robust  
346 prediction model, the calibration dataset should be sufficiently rich in variations,  
347 particularly taking into account the existing variability with the fruit itself ([Zhang et  
348 al., 2018](#)). Our prediction results provided advanced knowledge to determine where  
349 and how many positions are needed with the non-destructively NIRS measurements  
350 on apple surfaces, as well as to access the sample portion to be analyzed by reference  
351 methods for the calibration set.

352 In the literature, NIR predictions of apple quality traits involve taking  
353 measurements at up to four points located in the equatorial region ([Liu and Ying, 2005](#);  
354 [Peirs et al., 2003](#); [Pissard et al., 2012](#)), or along the stem, equator and calyx positions  
355 of apples ([Fan et al., 2016](#)). However, there was a reverse conclusion to reach the  
356 accurate predictions of developed models following each of these two methods. From  
357 our results, a specific attention needs to be paid according to the ‘cultivar’, which is  
358 the major factor influencing the fruit heterogeneity and the possible reason to explain  
359 the aforementioned disagreement result. According to the relative standard deviation  
360 (RSD) values of the predicted DMC and TSC of all pixels in single apples, different

361 levels of internal chemical variations were observed in Braeburn (RSD of DMC =  
362 24.6 % and of TSC = 22.1 %), Royal Gala (RSD of DMC = 26.5 % and of TSC =  
363 27.1 %), Granny Smith (RSD of DMC = 18.9 % and of TSC = 22.0 %) and thinned  
364 Golden Delicious (RSD of DMC = 13.2 % and of TSC = 15.7 %). These results  
365 indicated the same and limited spectral measurement points for all apples could not  
366 present such intensive internal quality variations of different cultivars. From a  
367 spectroscopic point of view, an increase of measured positions on apple surfaces  
368 therefore is particularly important to improve accuracy in the calibration steps.

369 In all apples, the large DMC and TSC differences among the middle (the average  
370 predicted DMC of all pixels in slice C and D of all cultivars =  $136.5 \pm 16.2$  g/kg and  
371 TSC =  $115.6 \pm 14.3$  g/kg), top (the average predicted DMC of all pixels in slice A and  
372 B of all cultivars =  $117.1 \pm 22.4$  g/kg and TSC =  $79.5 \pm 17.1$  g/kg) and bottom slices  
373 (the average predicted DMC of all pixels in slice E and F of all cultivars =  $124.1 \pm$   
374  $25.2$  g/kg and TSC =  $87.3 \pm 20.1$  g/kg) demonstrated that four points at the equatorial  
375 region might not be enough to provide the representative spectra of the entire apple  
376 fruit. NIRS information from top to bottom of apple surfaces therefore needs to be  
377 considered for all apple cultivars.

378 Consequently, the strong variability and heterogeneity of apples were highlighted  
379 using our developed models, and probably constitute the major barrier to an accurate  
380 NIR modelling. The similar distribution results of TSC and DMC in apple slices were  
381 observed in most apple slices of each cultivar (at least 4 over 6 fruits). These results  
382 provided an important opportunity to advance our knowledge on the quality

383 measurement: where and how many specific positions need to be measured on apple  
384 surfaces with NIRS, in order to develop accurate and robust prediction models.

385 The previous HSI models mainly detected the soluble solids content and firmness  
386 changes in single fruit (Mo et al., 2017; Sun et al., 2017), because of the quick and  
387 easy reference data quantification of all targeted samples using digital refractometers  
388 and hardness detectors. Compared to these studies, our work provided an efficient  
389 solution for the HSI modelling calibration step, depending on the reference data  
390 measured on 141 representative samples instead of the 1056 prepared samples.  
391 Importantly, this method offered a new sight on contents of total sugars (sum of the  
392 fructose, glucose and sucrose) and dry matter in apples, with a limited number of  
393 complicated (individual sugars measured by spectrometry using enzymatic kits) and  
394 time-consuming (at least 24 hours for freeze-drying) analyses for HSI modelling. In  
395 future, such a rapid and efficient approach for HSI modelling calibration would be  
396 helpful to detect the variations of apple internal quality parameters according to  
397 different environmental conditions (crop load, irrigation, light penetration and  
398 elevations of regions etc.—) and growing stages, and then contribute to an  
399 improvement of apple quality and production. The objective at the end could be to  
400 have a better knowledge of the apple homogeneity in order to manage them better for  
401 fresh market and processing taking into account the sustainability of practices.

#### 402 **4. Conclusion**

403 In this study, the power of chemometric methods was harnessed in a two-steps  
404 procedure for mapping of apple fruit heterogeneity while minimizing the number of

405 chemical analyses. PCA of NIR-HSI data was used to scan the heterogeneity of apple  
406 slices and to pin-point the best representing areas of the whole spectral variation. A  
407 limited number of chemical measurements could then be carried out and exploited by  
408 PLS regression to identify the underlying compositional information present in  
409 NIR-HSI data at individual pixels. NIR-HSI coupled with PLS regression showed a  
410 good ability to phenotype the distribution of dry matter content and total sugars  
411 content in apple fruit. The prediction models developed with the reference values of  
412 the most variable areas identified by PCA on HSI data were enough to assess the  
413 variability and heterogeneity of apple global parameters, with acceptable precisions  
414 (range of values). For dry matter and total sugars, the PLS results had a better ability  
415 than the random forest ones to estimate their distributions in apple slices. With the  
416 rapid scanning of apple slices and a limited number of chemical measurements, this  
417 method showed the great advantages of a simple fruit sampling, less experimental  
418 deviations caused by rapid oxidation of fruit, and a high efficiency of model  
419 developments. This method opens the possibility to more systematically evaluate the  
420 fruit variability and heterogeneity in future projects.

#### 421 **Acknowledgements**

422 The authors thank Shouyang Liu, Xiuliang Jin, Jiantao Zhao, Patrice Reling,  
423 Barbara Gouble, Line Touloumet, Marielle Boge, Caroline Garcia (INRAE, SQPOV  
424 unit) for their technical help. The ‘Interfaces’ project is an Agropolis Fondation  
425 Flashship project publicly funded through the ANR (French Research Agency) under  
426 “Investissements d’Avenir” programme (ANR-10-LABX-01-001 Labex Agro,

427 coordinated by Agropolis Fondation). Weijie Lan was supported by a doctoral grant  
428 from Chinese Scholarship Council.

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547

548 **Figure captions:**

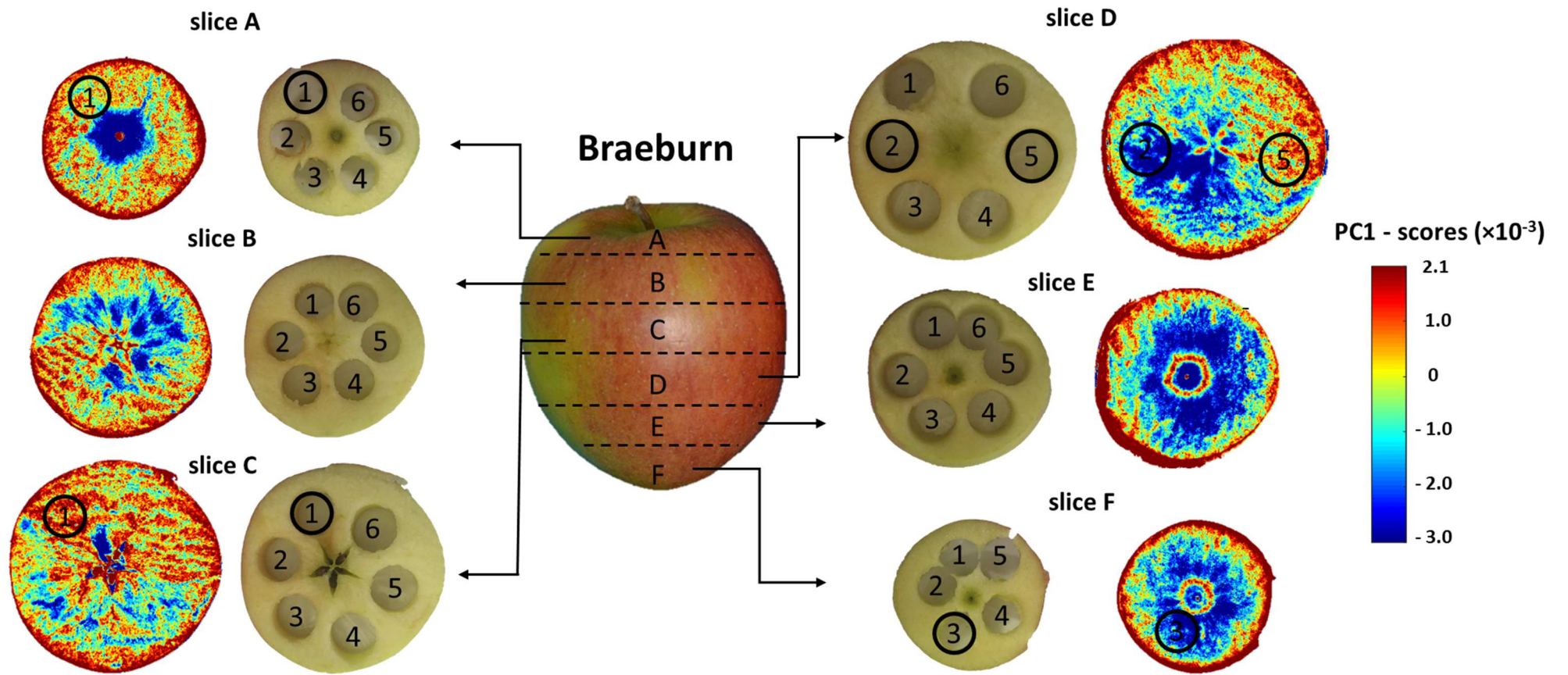
549 **Fig. 1.** The photographs of Braeburn apple slices and the first principal component  
550 (PC1) score (from the PCA results on all apple groups) plot of all near-infrared  
551 hyperspectral pixels (990- 2450 nm) for each slice (A, B, C, D, E, F). The selected  
552 ROIs were labelled with black circles.

553 **Fig. 2.** The boxplots of: (a) dry matter, (b) total sugars, (c) fructose, (d) sucrose, (e)  
554 glucose, (f) malic acid, (g) sum of polyphenols of ‘Braeburn’ (BR); ‘Granny Smith’  
555 (G□); ‘Royal Gala’ (GA); thinned ‘Golden Delicious’ (GD Th+) and non-thinned  
556 ‘Golden Delicious’ (GD Th-) apples.

557 **Fig. 3.** Comparison of the measured and the full-cross validated (a) dry matter content  
558 (DMC) and (b) total sugars content (T□C) of the 141 ROI samples; and the most  
559 contributing wavelengths for (c) DMC and (d) TSC prediction, using the  
560 leave-one-out PLS regression on the ROI averaged spectra.

561 **Fig. 4.** The distribution of total sugars content (TSC) in apple slices predicted by the  
562 LOO- PLS models developed based on the ROI averaged spectra.

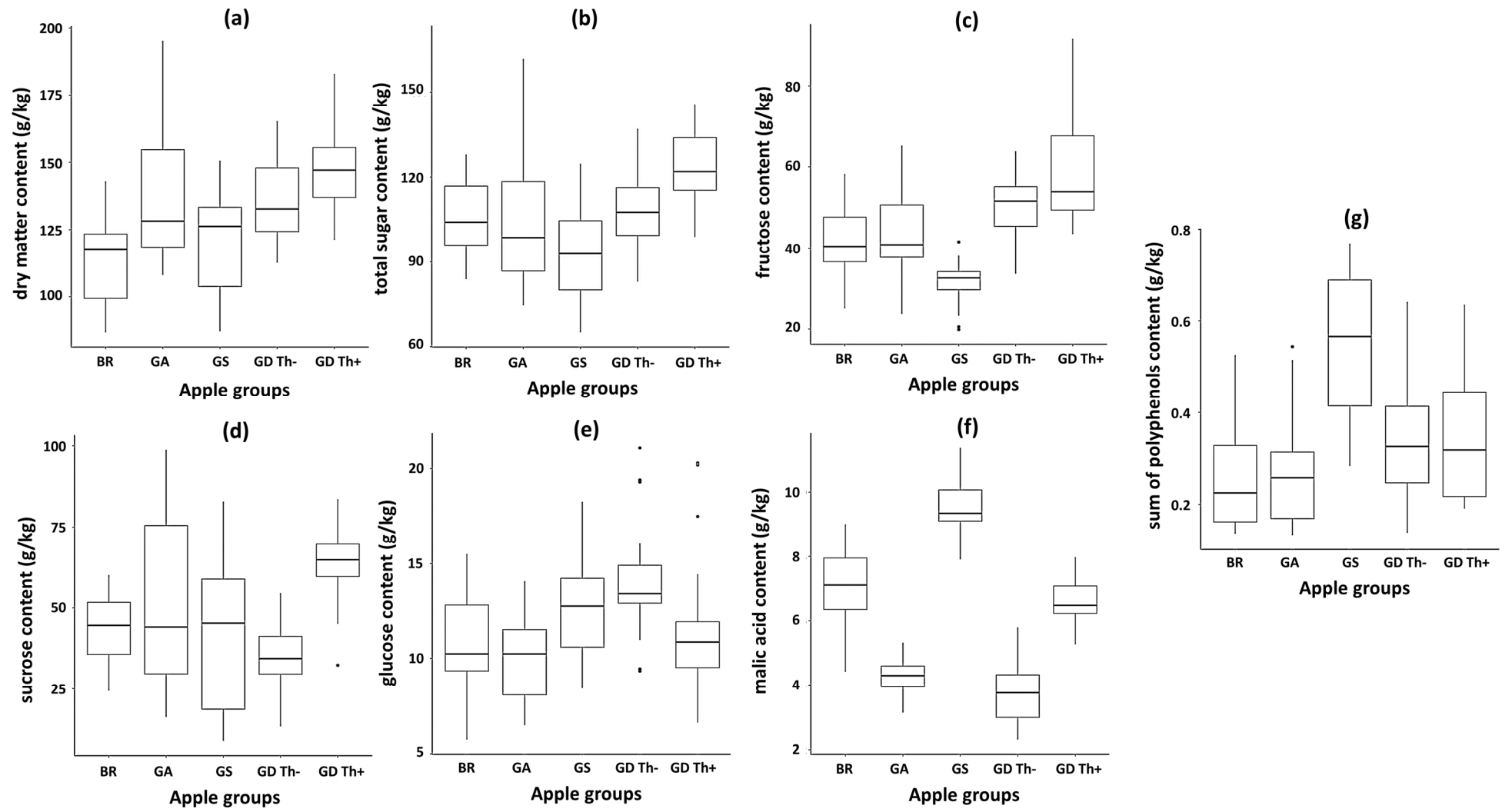
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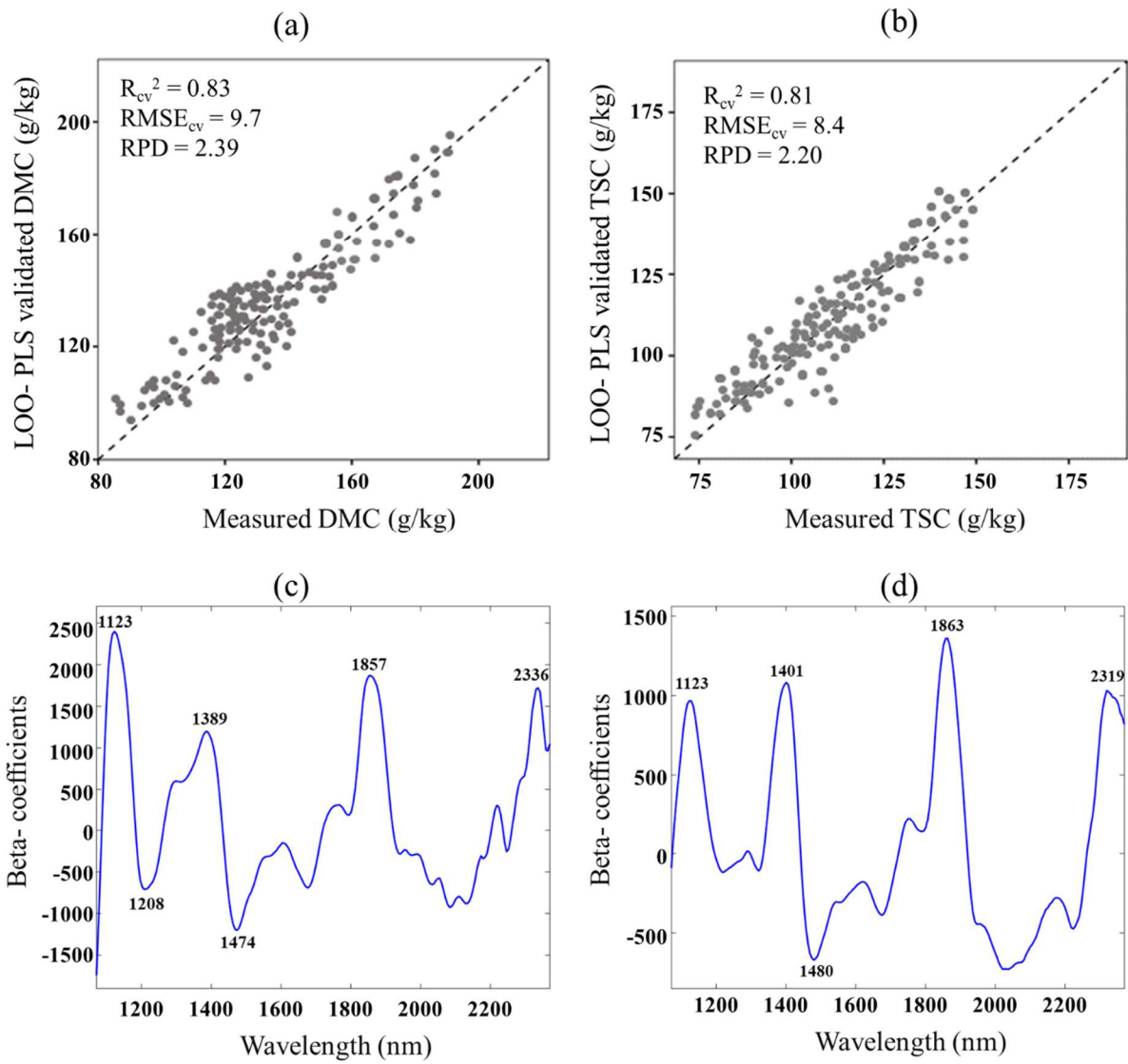
**Fig. 1**



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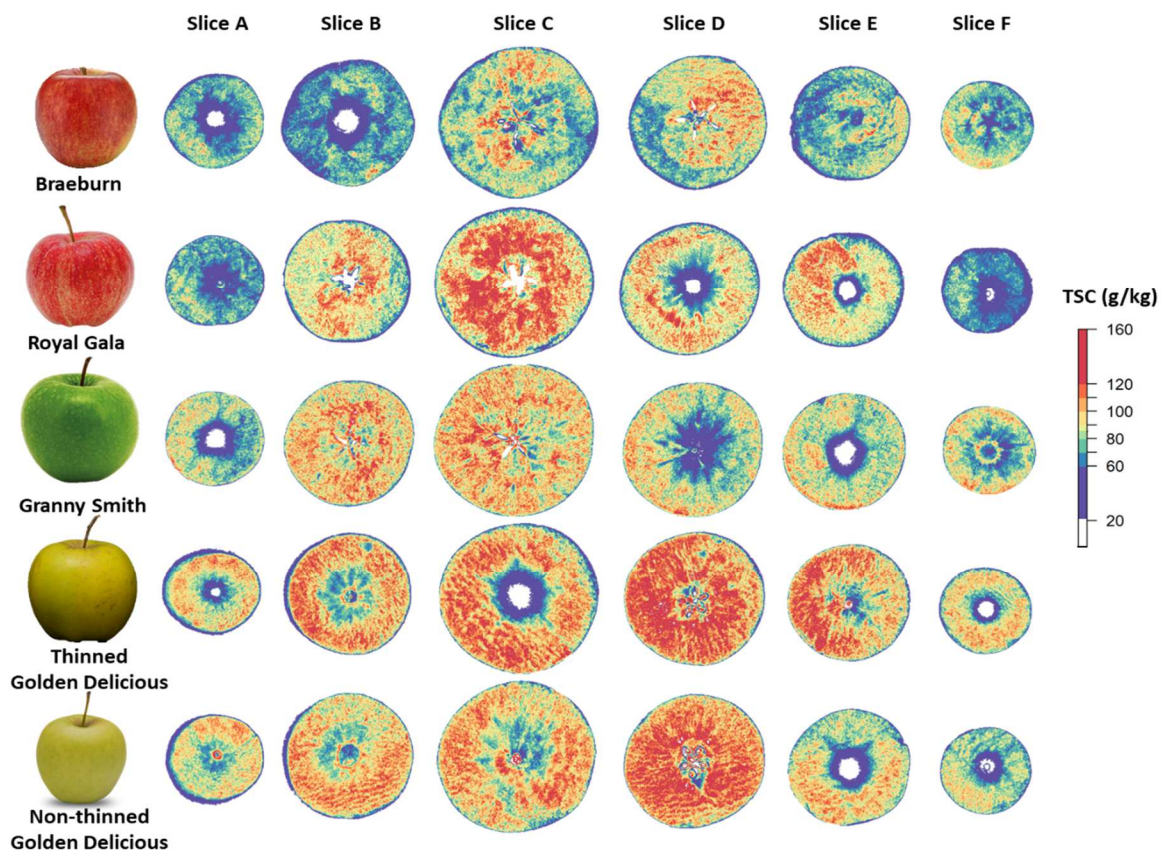
567

**Fig. 2**



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**Fig. 3**



570

571

**Fig. 4**

572 **Table 1** Leave- one- out partial least square (LOO-PLS) and random forest (RF) results of apple internal quality traits using the averaged  
 573 spectra of ROIs.

Parameters	Measured range	SD	Models	Full-crossed validation (n = 141)			
				R <sub>cv</sub> <sup>2</sup>	RMSE <sub>cv</sub>	RPD	LVs
dry matter (mg/g)	86.2- 195.3	21.9	PLS	0.83	9.7	2.39	7
			RF	0.67	14.8	1.58	7
total sugars content (g/kg)	58.8- 156.8	18.7	PLS	0.81	8.4	2.20	5
			RF	0.78	9.2	2.11	4
fructose (g/kg)	19.8- 91.6	15.4	PLS	0.38	9.0	1.35	9
			RF	0.32	10.1	1.24	8
sucrose (g/kg)	9.1- 98.7	8.4	PLS	0.67	4.9	1.73	8
			RF	0.65	5.8	1.40	6
glucose (g/kg)	5.7- 21.1	3.0	PLS	0.29	2.5	1.19	6
			RF	0.27	2.5	1.18	6
malic acid (g/kg)	2.3- 11.4	2.2	PLS	0.31	2.1	1.23	7
			RF	0.15	2.3	1.08	8
Sum of polyphenols (g/kg)	0.13- 0.77	0.16	PLS	0.14	0.17	1.01	8
			RF	0.13	0.21	0.85	9

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575

# Graphical abstract

