



Short communication

Feasibility of pocket-sized near-infrared spectrometer for the prediction of cheese quality traits

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ABSTRACT

This study aimed to evaluate the feasibility of a low-cost pocket-sized near-infrared spectrometer (NIR; 740–1070 nm) to predict cheese total nitrogen (%), soluble nitrogen (%), ripening index (%), major minerals (g/100 g of cheese), and fatty acids (g/100 g of cheese). A total of 104 ground cheeses samples were scanned 5 times with a pocket-sized NIR and matched with the reference data to develop the prediction models. Modified partial least squares regressions were developed and parameters were optimized through a leave one out cross-validation. Models were validated using 13-fold nested cross validation. The best models were obtained for total fatty acids (ratio of prediction to deviation, RPD = 6.61) and total nitrogen (RPD = 5.95) content. Regarding mineral content, best prediction models were obtained for P (RPD = 4.04), Na (RPD = 3.12), and Ca (RPD = 2.77). Main individual fatty acids and fatty acid groups were poorly predicted, except for SFA (RPD = 2.92), C16:0 (RPD = 2.83), and C4:0 (RPD = 2.51). However, the accuracy of the models was similar to those obtained with benchtop infrared devices. Thus, these results demonstrated that miniaturization of the NIR instruments represents an opportunity in the dairy industry.

1. Introduction

The dairy industry routinely uses infrared spectroscopy to predict gross composition (fat, protein, and humidity) of the products because it offers a quick, easy to manage, low cost, non-destructive, and chemical-free analysis, and is able to determine several traits concurrently. However, benchtop near-infrared (NIR) spectrometers require an important initial investment and cost of maintenance that is not always affordable by cheese manufacturers (De Marchi et al., 2018). Moreover, these benchtop NIR cannot be moved among facilities located in different places, therefore dairy companies need to purchase instruments at each site or to send samples to a centralized laboratory.

Recently, economic miniaturized portable NIR devices with a reasonable performance have arrived to the market and some studies have been conducted to evaluate their accuracy in vegetal and animal products (Liu et al., 2018; Ma et al., 2019). For example, portable NIR devices applied in the carcass surface has been tested in slaughterhouses revealing promising results (Kademi et al., 2019). Moreover, the advantage of some of these miniaturized devices is that they work in

cloud-based environments, where spectra and prediction models are stored, making it easy to obtain results in a user-friendly interface for food industry technicians (Wiedemair et al., 2019).

Cheese is known as a complex matrix due to the great variability of products on the market (hard, semi-hard, and soft cheese varieties) and the heterogeneity of the product itself (migration of components across the wheel, surface-center), which leads to build prediction models with a moderate to low accuracy depending on the trait (De Marchi et al., 2018). However, there is still scarce literature dealing with the accuracy of these economic miniaturized portable NIR devices in cheese, especially for quantitative determination of detailed composition.

Therefore, the aim of the present study was to evaluate the feasibility of a low-cost pocket-sized NIR spectrometer to predict total nitrogen (%), soluble nitrogen (%), ripening index (%), major minerals (g/100 g of cheese), and fatty acids (g/100 g of cheese) content in soft and semi-hard cheeses.

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2. Material and methods

2.1. Cheese samples and chemical analysis

A total of 104 ground cheeses samples from 8 soft and semi-hard cheese varieties (i.e., Caciotta, Mozzarella, Mozzarella Pizza, Primo sale, Ricotta siero, and Scarmorza) were purchased in the supermarket as well as provided by Sabelli Spa (Ascoli Piceno, Ascoli, Italy). The categorization of soft (> 45 % of water) and semi-hard (35 %–45 % of water) cheese is based on their moisture content (CLAL, 2018). Samples arrived refrigerated (4 °C) to the laboratory of the Department of Agronomy, Food, Natural resources, Animals, and Environment of the University of Padova (Legnaro, Italy) for the analysis. Each cheese sample was homogenized with a knife mill Retsch Grindmix GM200 (Retsch GmbH & Co, Haan, Germany). Grounded samples were kept in a sealed plastic bag at 4 °C and analyzed within 2 h to avoid variations in cheese composition depending on moisture loss.

Cheese moisture, protein, and fat content were determined using FoodScan™ Dairy Analyzer (Foss, Electric A/S, Hillerød, Denmark) through FOSS Artificial Neural Networks Dairy Calibration. The ripening index was calculated as WSN/TN, where the amount of total nitrogen (TN) and water-soluble nitrogen (WSN) were determined by the Kjeldahl method using a Tecator Kjeltak™ 2300 Analyzer Unit (Foss, Electric A/S, Hillerød, Denmark) according to the official method (Gazzetta Ufficiale n.229, 1986).

Fatty acids (FA) were quantified as described by (Manuelian et al., 2017a). Briefly, total lipids were extracted by an accelerated solvent extraction method using a Dionex ASE 350 system (Thermo Scientific, Dreieich, Germany) with petroleum ether as solvent (AOAC method #960.39) (International AOAC, 2016). Total fatty acids content was determined after solvent evaporation and expressed as a percentage. Fatty acid methyl esters of total lipids were prepared with an internal method adapted from (Christie, 1993). Separation and quantification of fatty acid methyl esters were performed using an Agilent 7820A GC System equipped with an automatic sampler G4567A (Agilent Technologies, Santa Clara, CA, USA) and a flame ionization detector. The individual fatty acids were identified by comparing their retention times with those of a standard fatty acid (Supelco FAME mixC4–C24 #18919-1AMP; Sigma-Aldrich). Peaks areas were calculated using GC/MSD ChemStation Software (Agilent Technologies) and expressed as percentage of total fatty acids. The FA groups were defined according to (Manuelian et al., 2017a).

Content of major minerals in cheese was quantified according to the method proposed in (Manuelian et al., 2017a), using inductively coupled plasma optical emission spectrometry (ICP-OES) Arcos EOP (SPECTRO Analytical Instruments GmbH, Kleve, Germany) following AOAC method #2013.06 (International AOAC, 2016). The calibration solutions for each mineral were prepared from single element solutions (Inorganic Ventures, Christiansburg, VA, USA) in a concentration range between 0 and 100 mg/L. Minerals were expressed in g/100 g of the raw product.

2.2. Spectral collection and chemometric analysis

Each grounded sample was scanned in 5 locations with a pocket-sized NIR (67.7 × 40.2 × 18.8 mm; SCiO™) every 1 nm from 740 to 1070 nm at room temperature and absorbance was recorded as log (1/reflectance). Predictions were built using modified partial least squares regression analysis (WinISI III v. 1.60; Foss and Infrasoft International LLC, State College, PA) through a leave one out cross-validation. Several combinations of scattering correction (no correction, NONE; detrend, DET; standard normal variate, SNV; SNV + DET, SND; and standard multiplicative scatter correction, MSC) and derivative (0,0,1,1; 1,4,4,1; 1,8,8,1; 2,5,5,1; and 2,10,10,1, where the first digit representing the number of the derivative, the second the gap over which the derivative is calculated, the third the number of data points in the first smoothing,

and the fourth the number of data points in the second smoothing) were tested. The number of latent variables included in the model were selected according to van der Voet (1994).

To improve the accuracy of the models, before each regression the scans were separately evaluated for Mahalanobis distance and the ones with GH > 3 were eliminated. Remaining scans were averaged within each sample and regression was performed. Afterwards, chemical outliers (T values > 3) were removed and outlier elimination passes were iterated three times (Soyeurt et al., 2012). The best prediction equation was chosen with respect to the number of latent factors (LF); the standard error of calibration (SE_C) and cross-validation (SE_{CV}); the coefficient of determination of calibration (R²) and cross-validation (R²_{CV}). Moreover, in order to assess reliable performance statistics for developed calibration, an outer 13-fold cross-validation (nested validation) was performed maintaining previously optimized parameter (i.e. number of latent variables, mathematical treatment, scatter correction, samples included in dataset) (Krstajic et al., 2014). Calculated performance statistics were coefficient of determination of nested validation (R²_{NV}), standard error of nested validation (RMSE_{NV}) and ratio of prediction to deviation (RPD), calculated as the ratio of the SD of the trait to the SE_{NV} (Williams, 2014; Williams and Sobering, 1993).

3. Results & discussion

The descriptive composition of the ground cheese samples employed for the development of the calibration equations in this study is reported in Tables 1 and 2. Different varieties of soft and semi-hard cheese were included to provide a broad range in the traits evaluated, which is considered a basic principle to obtain good calibration models (Naes et al., 2002). The lowest coefficient of variation was observed for the moisture content, which was expected because only soft and semi-hard cheese varieties were included.

Average absorbance spectra for ground cheese samples obtained with the pocket-sized NIR device is shown in Fig. 1. Although the pocket-sized NIR used in the present study covered a narrow wavelength range, the average NIR raw spectrum obtained followed a similar shape to those previously collected from cheese samples (Lucas et al., 2008). Spectra were also in agreement with the one reported in intake cheese samples (Wiedemair et al., 2019). The wide peak observed between 940 nm and 1050 nm has been attributed to OH second overtone and described in intact cheese samples (Wiedemair et al., 2019). In particular, a greater absorbance at about 982 nm has been attributed to water (Kays et al., 2000) and described previously in cheese (Lucas et al., 2008).

Table 1
Descriptive statistics^a of cheese composition, ripening index and mineral content.

Trait	N	Media	SD	CV	Minimum	Maximum
Composition traits (%)						
Moisture	104	64.35	10.66	16.56	39.48	75.70
Fat	104	18.14	6.63	36.57	7.49	32.95
Protein	104	12.72	5.39	42.39	5.87	23.20
Nitrogen related traits (%)						
Total nitrogen	104	2.31	0.87	37.73	1.31	4.22
Soluble nitrogen	104	0.30	0.16	53.44	0.06	0.82
Ripening Index	104	12.67	4.60	36.30	4.52	24.89
Minerals (g/100 g)						
Ca	104	0.45	0.16	36.63	0.22	0.75
K	104	0.08	0.04	50.79	0.02	0.14
Mg	104	0.03	0.02	80.64	0.01	0.08
Na	104	0.26	0.17	65.51	0.04	0.69
P	104	0.30	0.12	38.27	0.16	0.53

^a N: Number of analyzed samples; SD: Standard deviation; CV: coefficient of variation.

Table 2Descriptive statistics^a of cheese main fatty acids.

Trait ^b (g/100 g)	N	Media	SD	CV	Minimum	Maximum
Fatty acids	104	17.14	6.27	36.57	7.07	31.14
SFA	103	12.14	4.57	37.64	4.82	24.34
C4:0	103	0.45	0.21	46.95	0.03	1.00
C6:0	103	0.30	0.16	54.15	0.02	0.71
C8:0	103	0.20	0.10	49.42	0.013	0.45
C10:0	103	0.47	0.24	50.93	0.03	1.08
C12:0	103	0.57	0.30	53.49	0.03	1.34
C14:0	103	1.80	1.05	58.09	0.02	4.21
C15:0	103	0.22	0.10	43.95	0.02	0.47
C16:0	103	5.70	2.60	45.58	0.12	12.24
C18:0	103	1.82	0.99	54.42	0.12	4.44
MUFA	103	4.26	2.23	52.38	0.64	8.73
C14:1	103	0.16	0.09	55.30	0.011	0.41
C16:1	103	0.28	0.16	56.19	0.01	0.63
C18:1	103	3.27	1.98	60.71	0.16	7.05
C18:1 c	103	0.30	0.18	60.80	0.02	0.78
PUFA	103	0.77	0.32	41.86	0.15	1.63
□-3	103	0.15	0.07	46.54	0.03	0.38
C18:3	103	0.08	0.05	59.39	0.004	0.23
C18:4	88	0.007	0.007	94.09	0.001	0.05
C20:3	98	0.04	0.014	37.47	0.015	0.08
C20:5	96	0.010	0.008	77.87	0.002	0.06
C22:6	103	0.02	0.02	90.23	0.004	0.14
□-6	103	0.53	0.24	46.61	0.06	1.05
C18:2	103	0.47	0.23	49.26	0.03	0.96
C18:2 t	61	0.007	0.004	54.20	0.001	0.02
C18:3	101	0.010	0.005	54.91	0.001	0.03
C20:2	102	0.011	0.005	46.11	0.004	0.03
C20:3	103	0.02	0.009	37.02	0.008	0.05
C20:4	49	0.004	0.003	73.94	0.001	0.02
C22:2	44	0.009	0.006	60.24	0.003	0.03

^a N: Number of analyzed samples; SD: Standard deviation; CV: coefficient of variation.

^b SFA: Saturated fatty acids; MUFA: Monounsaturated fatty acids; PUFA: Polyunsaturated fatty acids; □-3: omega-3 fatty acids; □-6: omega-6 fatty acids.

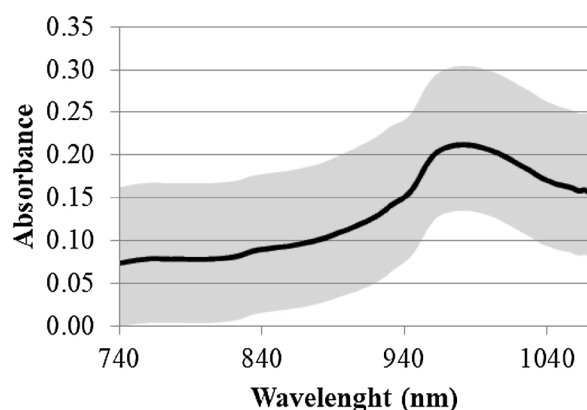


Fig. 1. Mean of collected spectra (black line). Gray shadow represents $\pm$ wavelengths standard deviation.

Spectral outlier elimination (GH outliers) was performed before averaging scans for regression. This was decided considering spectra acquisition is not standardized as in benchtop instruments. In particular, the angle between the spectrometer and the sample, their relative distance, and the exposure to different external conditions are potential sources of interferences (Beć et al., 2021). The inclusion of abnormal scans during spectra averaging can potentially affect regression in two ways: (i) averaged spectrum is not detected as an outlier even if it carries poor quality scans, affecting prediction model quality; (ii) averaged spectrum is recognized as outlier, even if 4 out of 5 scans were correctly recorded, causing the loss of useful information.

Different derivatives of spectral data were tested for their ability to remove or reduce disturbing effects not related to the chemical

absorption of light. The model for each trait shown in Tables 3 and 4 is the best result from 25 models resulting from the evaluation of different derivatives (5 scatter correction techniques and 5 math treatments).

Calibration for total nitrogen revealed good performances, with R^2_{NV} (0.97) and RPD (5.95), which indicates that the calibration model built can be used for any application (Karoui et al., 2006a; Williams, 2014). The accuracy of the models are in agreement with (Lin et al., 2014) who reported R^2 in prediction and RPD in intact cheese samples close to 0.98 and 5.6, respectively, using a field spectroradiometer. However, a pocket-sized NIR spectrometer reported lower accuracy of the model for total protein ($N \times 6.25$) content in grated Cheddar cheese samples with a RPD from 1.7 to 3.1 using different wavelength selection method and different preprocessing techniques (Ma et al., 2019). Compared with a laboratory NIR instrument, the accuracy of our model for soluble nitrogen was slightly lower than the one reported for different cheese varieties (Franzoi et al., 2021), but better than the one reported for Emmental cheese ($R^2_{CV} = 0.77$) (Karoui et al., 2006b). Based on Williams (2014) interpretation guidelines of RPD in complex matrices, the model we built was only adequate for a rough screening. A very poor calibration model (RPD = 1.34) was obtained for the prediction of the ripening index, which disagree with the results reported by Currò et al. (2017) when including a greater variability of cheese ripening time (RPD > 3.0). Thus, the differences in terms of accuracy observed for total nitrogen, soluble nitrogen, and ripening index could be explained by the range of variation considered in each study (De Marchi et al., 2018) instead of the instrument used.

To the best of our knowledge, pocket-sized NIR devices have not been evaluated to predict mineral and fatty acid content in cheese samples. However, several studies have been conducted using laboratory NIR instruments (De Marchi et al., 2018). Mineral calibrations are difficult to achieve because NIR spectroscopy could only detect minerals if they are in organic complexes (Buing-Pfaue, 2003; Woodcock et al., 2008), which explains the greater number of LF needed compared to the other traits evaluated. However, the LF we obtained were in agreement with previous studies conducted using laboratory spectrometers (Manuelian et al., 2017b, 2017a). As observed in Table 2, adequate calibration models for quantitative analysis were achieved for P and Na, revealing a RPD ≥ 3.0 , while RPD obtained for Ca can be considered adequate for screening purposes (Williams, 2014). Those results are in agreement with the ones reported using NIR in transmittance mode when including several soft to hard cheese varieties (Manuelian et al., 2017a) and better than the ones obtained with a fiber optic probe (González-Martín et al., 2011). The lower accuracy obtained for K and Mg could be related to the lower amount of those minerals compared to P and Na (González-Martín et al., 2011).

Main individual fatty acids and groups presented very poor calibration models, even if they were expressed as total amount (Table 4) rather than as relative concentration. Calibration models with an RPD > 2.5 were only found for SFA, C4:0, and C16:0. These results were also in agreement with the ones reported using NIR in transmittance mode when including several soft to hard cheese varieties (Manuelian et al., 2017a).

4. Conclusion

The present study evaluated the prediction accuracy of a pocket-sized NIR with a narrow wavelength range (740–1070 nm) for total nitrogen, soluble nitrogen, ripening index, major minerals content (Ca, K, Mg, Na, and P), and fatty acid profile in soft and semi-hard cheese varieties. The average spectra recorded with the pocket-sized NIR, which worked with a narrow wavelength range (740–1070 nm), was similar to the ones described in the literature for benchtop NIR devices. The best prediction models were built for total fatty acids ($RPD_{NV} = 6.61$), total nitrogen ($RPD_{NV} = 5.95$), P ($RPD_{NV} = 4.04$), Na ($RPD_{NV} = 3.12$), and Ca ($RPD_{NV} = 2.77$), SFA ($RPD_{NV} = 2.92$), C16:0 ($RPD_{NV} = 2.83$), and C4:0 ($RPD_{NV} = 2.51$). These results suggested that the

Table 3

Fitting statistics of calibration, cross-validation, and nested validation results^a for cheese nitrogen content, soluble nitrogen fraction, ripening index, and mineral content using portable-NIR.

Trait	N	Math	LF	SE _c	R ²	SE _{cv}	R ² _{cv}	SE _{nv}	R ² _{nv}	RPD _{nv}
Nitrogen related traits (%)										
Total nitrogen	500	SNV1881	9	0.80	0.98	0.89	0.97	0.91	0.97	5.95
Soluble nitrogen	504	MSC1441	7	0.40	0.83	0.46	0.78	0.46	0.78	2.15
Ripening index	509	NO1441	8	2.86	0.59	3.21	0.48	3.40	0.44	1.34
Minerals (g/100 g)										
Ca	506	MSC0011	12	0.05	0.89	0.06	0.87	0.06	0.87	2.77
P	509	SND1881	7	0.03	0.95	0.03	0.94	0.03	0.94	4.04
K	512	NO1881	9	0.02	0.82	0.02	0.78	0.02	0.77	2.07
Mg	509	NO1441	7	0.009	0.82	0.010	0.78	0.01	0.78	2.13
Na	511	MSC0011	11	0.05	0.92	0.06	0.90	0.05	0.90	3.12

^a N: number of spectra after outlier removal; Math: derivative (derivative order, subtraction gap, first smoothing, second smoothing) and scatter correction (SNV: standard normal variate; DET: detrend; SND: SNV + DET; MSC: standard multiple scatter correction) of the spectra; LF: number of latent factors; SE_c: standard error in calibration; R²: coefficient of determination in calibration; SE_{cv}: standard error in cross validation; R²_{cv}: coefficient of determination in cross validation; RPD: ratio of prediction to deviation.; SE_{nv} = standard error in nested validation; R²_{nv} = coefficient of determination in nested validation.

Table 4

Fitting statistics for calibration, cross-validation, and nested validation results^a for total, saturated, monounsaturated and polyunsaturated fatty acids using portable-NIR.

Trait (g/100 g) ^b	N ^a	Math	LF	SE _c	R ²	SE _{cv}	R ² _{cv}	SE _{nv}	R ² _{nv}	RPD _{nv}
Fatty acids										
SFA	494	SNV0011	6	1.44	0.89	1.52	0.88	1.51	0.88	2.92
C4:0	472	SND2551	2	0.07	0.86	0.07	0.84	0.07	0.84	2.51
C6:0	474	DET2551	2	0.07	0.78	0.07	0.76	0.07	0.76	2.06
C8:0	477	NO0011	4	0.04	0.76	0.05	0.74	0.05	0.74	1.98
C10:0	470	DET210101	2	0.10	0.77	0.11	0.76	0.11	0.76	2.04
C12:0	472	NO0011	5	0.14	0.76	0.14	0.73	0.23	0.41	1.30
C14:0	476	DET210101	2	0.55	0.69	0.57	0.67	0.57	0.67	1.74
C15:0	473	NO2551	4	0.03	0.83	0.04	0.80	0.04	0.79	2.17
C16:0	463	SND0011	7	0.71	0.90	0.79	0.87	0.78	0.87	2.83
C18:0	451	MSC2551	1	0.62	0.43	0.64	0.40	0.70	0.39	1.28
MUFA										
	459	MSC2551	1	1.28	0.60	1.32	0.58	1.33	0.58	1.54
C14:1	466	SND1441	4	0.04	0.73	0.05	0.69	0.05	0.69	1.79
C16:1	482	DET2551	4	0.07	0.79	0.07	0.75	0.08	0.73	1.93
C18:1 c	459	SND2551	1	0.12	0.52	0.12	0.49	0.12	0.49	1.40
C18:1	483	DET1441	2	1.18	0.64	1.21	0.62	1.20	0.62	1.63
PUFA										
	499	NO210101	2	0.20	0.60	0.20	0.57	0.20	0.57	1.53
□ -3	492	DET210101	2	0.04	0.54	0.04	0.50	0.04	0.50	1.41
C18:3	433	SND210101	1	0.02	0.68	0.02	0.67	0.02	0.66	1.71
C18:4	421	NO2551	6	0.002	0.71	0.003	0.62	0.003	0.56	1.52
C20:3	475	MSC1881	3	0.01	0.71	0.01	0.67	0.01	0.66	1.71
C20:5	435	SND1441	7	0.004	0.57	0.004	0.44	0.004	0.33	1.23
C22:6	462	SND1441	4	0.004	0.63	0.004	0.55	0.005	0.51	1.42
□ -6	487	DET1881	2	0.17	0.52	0.17	0.50	0.17	0.49	1.40
C18:2	489	MSC0011	2	0.16	0.52	0.16	0.49	0.16	0.49	1.40
C18:2 t	270	SND2551	1	0.002	0.37	0.002	0.28	0.003	0.39	1.29
C18:3	492	MSC210101	4	0.003	0.56	0.003	0.46	0.004	0.35	1.24
C20:2	507	MSC1441	3	0.004	0.48	0.004	0.39	0.004	0.33	1.22
C20:3	501	SND210101	2	0.005	0.68	0.01	0.64	0.01	0.63	1.62
C20:4	215	MSC2551	1	0.001	0.58	0.001	0.51	0.002	0.38	1.27
C22:2	202	MSC0011	9	0.002	0.65	0.002	0.47	0.003	0.23	1.15

^a N: number of spectra after outlier removal; Math: derivative (derivative order, subtraction gap, first smoothing, second smoothing) and scatter correction (SNV: standard normal variate; DET: detrend; SND: SNV + DET; MSC: standard multiple scatter correction) of the spectra; LF: number of latent factors; SE_c: standard error in calibration; R²: coefficient of determination in calibration; SE_{cv}: standard error in cross validation; R²_{cv}: coefficient of determination in cross validation; RPD: ratio of prediction to deviation.; SE_{nv} = standard error in nested validation; R²_{nv} = coefficient of determination in nested validation.

^b SFA: Saturated fatty acids; MUFA: Monounsaturated fatty acids; PUFA: Polyunsaturated fatty acids; □-3: omega-3 fatty acids; □-6: omega-6 fatty acids.

accuracy of the traits evaluated using a pocket-sized NIR with a narrow wavelength range (740–1070 nm) are similar to benchtop devices. The lower accuracy observed could be related to the concentration of the parameter evaluated and the variability considered in the samples included and not to the miniaturization of the device itself. Thus, the results demonstrated that miniaturization of the NIR instruments represents an opportunity in the dairy industry.

Author statement

Carmen L. Manuelian: Writing - original draft, Writing - review &

editing. **Matteo Ghetti:** Methodology, Formal analysis. **Claudia De Lorenzi:** Methodology, Formal analysis. **Marta Pozza:** Methodology, Formal analysis. **Marco Franzoi:** Formal analysis, Writing - review & editing. **Massimo De Marchi:** Conceptualization, Supervision, Funding acquisition, review & editing.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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