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SUPPLEMENTARY MATERIAL

Spectroscopic control of fish products: simultaneous recognition of species and thawed status in large-scale distribution

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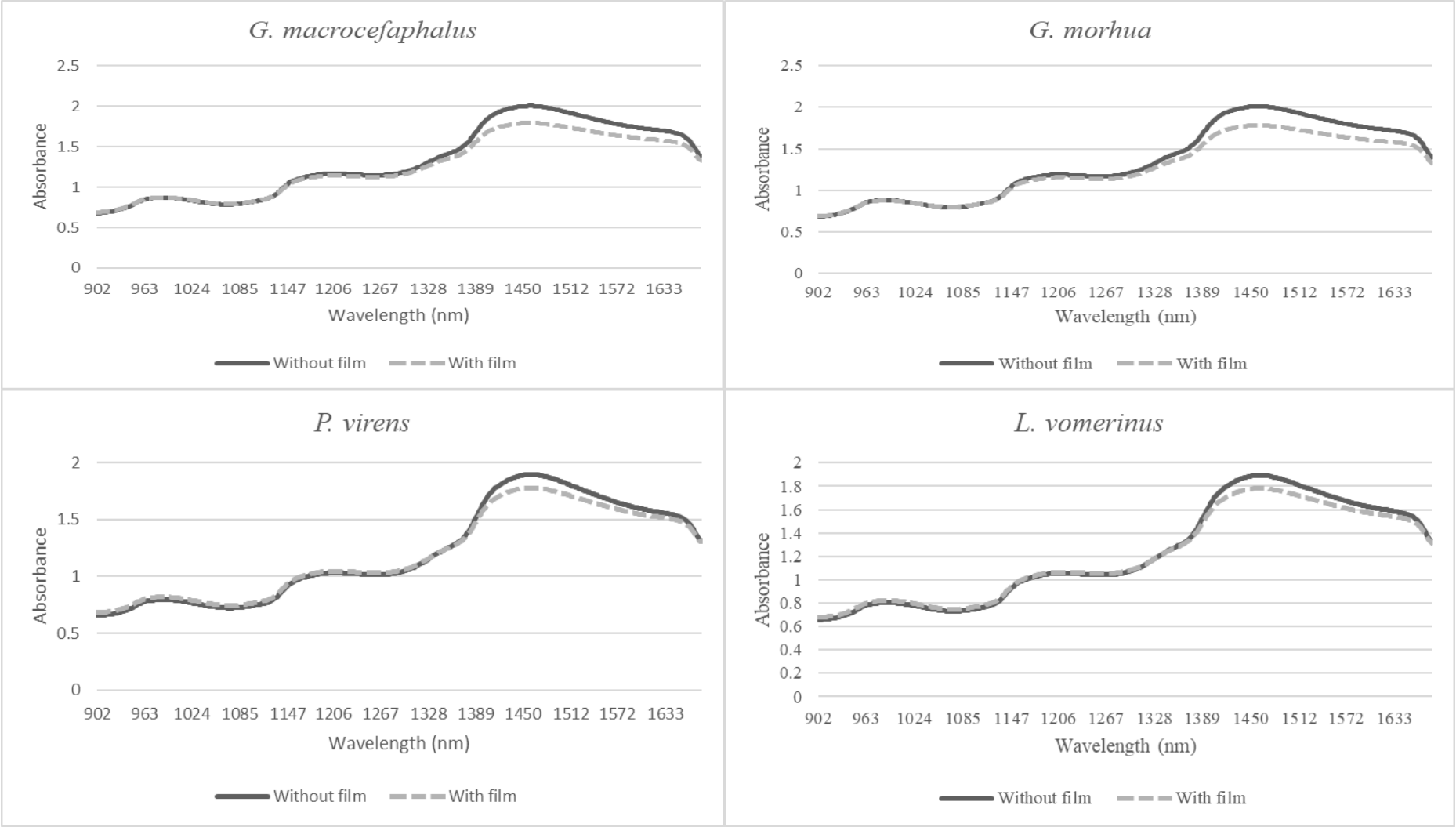
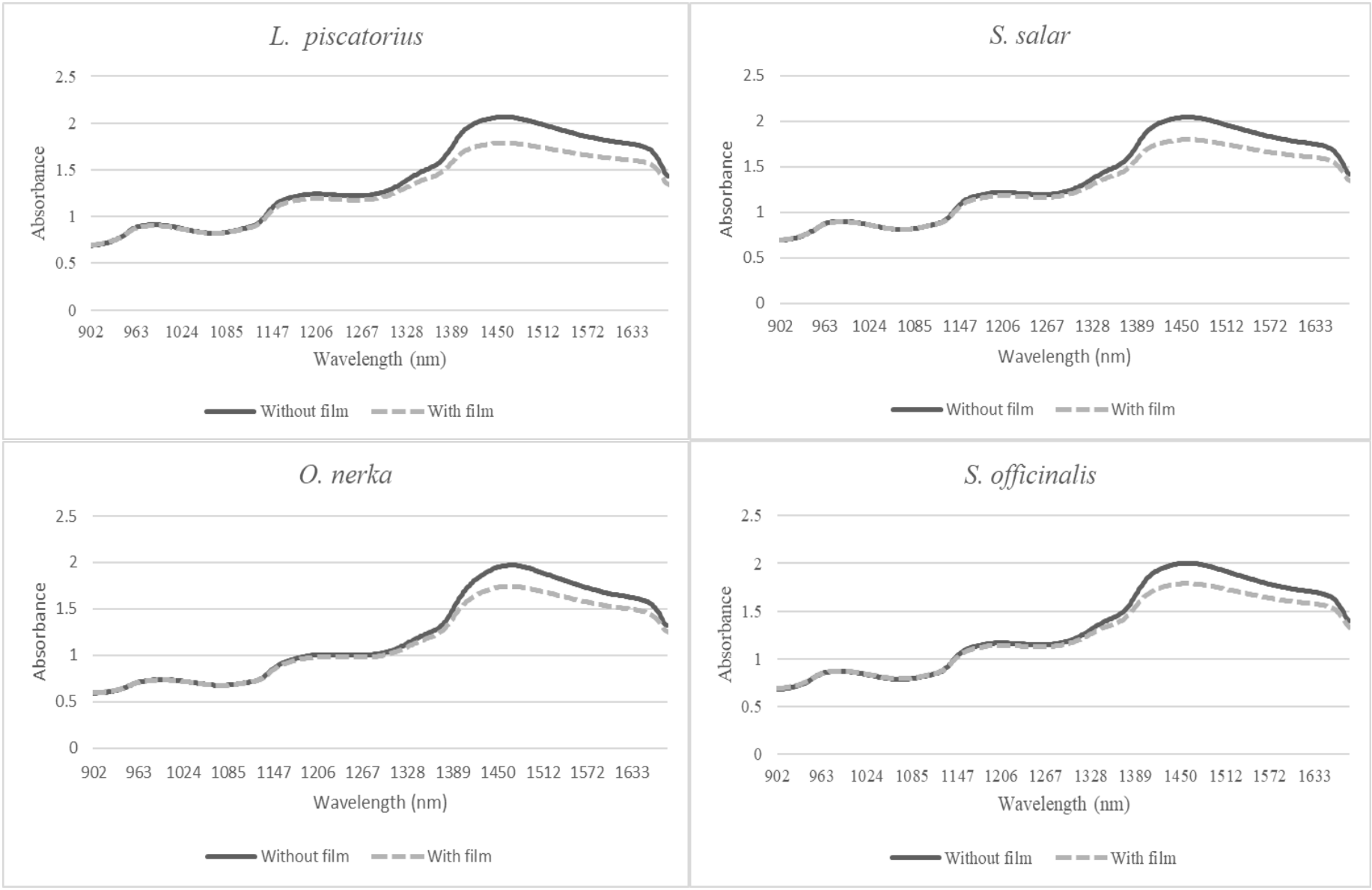
Key words: traceability, near infrared spectroscopy, seafood, film, classification.


G. macrocefaphalus
Absorbance
2.5
2
1.5
1
0.5
0
902 963 1024 1085 1147 1206 1267 1328 1389 1450 1512 1572 1633
Wavelength (nm)
Without film
With film
G. morhua
Absorbance
2.5
2
1.5
1
0.5
0
902 963 1024 1085 1147 1206 1267 1328 1389 1450 1512 1572 1633
Wavelength (nm)
Without film
With film
P. virens
Absorbance
2
1.5
1
0.5
0
902 963 1024 1085 1147 1206 1267 1328 1389 1450 1512 1572 1633
Wavelength (nm)
Without film
With film
L. vomerinus
Absorbance
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
902 963 1024 1085 1147 1206 1267 1328 1389 1450 1512 1572 1633
Wavelength (nm)
Without film
With film



Supplementary Figure 1. Graphical reconstruction of wavelength for the absorbance into the NIRS range of the eight species tested, both with and without film. The black line represents the spectral data acquired without film and the grey line represents the data with film.

Supplementary Table 1. **Samples collected description: samples were collected based on availability from large-scale retail outlets. For each specimen, the scientific and commercial name, and the number of fresh and frozen and thawed product analyses were reported (Ministero dell'agricoltura, 2020).**

Specie	Commercial name	Italian name	Fresh (no.)	Frozen-thawed (no.)	No. of point of sale	Origin
Sepia officinalis	Cuttlefish	Seppia	25	32	33	FAO 27
Salmo salar	Atlantic salmon	Salmone	47	/	34	FAO 27
Oncorhynchus nerka	Sockeye salmon	Salmone rosso	/	3	2	FAO 67
Lophius piscatorius	Angler	Rospo o Rana pescatrice	16	4	21	FAO 41 and FAO 27
Lophius vomerinus	Devil anglerfish	Rana pescatrice oceanica	/	11	6	FAO 47
Gadus macrocephalus	Pacific cod	Merluzzo nordico	1	40	32	FAO 27 and FAO 61
Gadus morhua	Atlantic cod	Merluzzo nordico	6	/	3	FAO 27
Pollachius virens	Pollock	Merluzzo carbonaro	33	/	14	FAO 27

Supplementary Table S2a. Support vector machine confusion matrix results with and without film investigating species using the hold-out (70-30%) and an internal cross-validation.

SVM Linear – Species identification with film								
	Reference							
Prediction	*G.macrocefaphalus*	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
G.macrocefaphalus	11	0	1	0	0	0	1	0
G.morhua	0	0	0	1	0	0	0	0
L.piscatorius	0	0	5	0	0	0	0	0
L.vomerinus	0	0	0	2	0	0	0	0
O.nerka	0	0	0	0	0	0	0	0
P.virens	0	0	0	0	0	7	1	0
S.officinalis	1	1	0	0	0	1	15	0
S.salar	0	0	0	0	0	1	0	14
SVM Linear Grid – Species identification with film								
	Reference							
Prediction	*G.macrocefaphalus*	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
G.macrocefaphalus	11	0	2	0	0	0	1	0
G.morhua	0	1	0	1	0	0	0	0
L.piscatorius	1	0	3	0	0	0	0	0
L.vomerinus	0	0	0	2	0	0	0	0
O.nerka	0	0	0	0	0	0	0	0
P.virens	0	0	0	0	0	8	1	0
S.officinalis	0	0	1	0	0	0	15	0
S.salar	0	0	0	0	0	1	0	14
SVM Linear – Species identification without film								
	Reference							
Prediction	*G.macrocefaphalus*	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
G.macrocefaphalus	11	0	1	0	0	0	1	0
G.morhua	0	0	0	0	0	0	1	0
L.piscatorius	0	0	3	0	0	0	0	0
L.vomerinus	0	0	0	3	0	0	0	0
O.nerka	0	0	0	0	0	0	0	0
P.virens	0	0	0	0	0	9	0	0
S.officinalis	1	1	2	0	0	0	15	0
S.salar	0	0	0	0	0	0	0	14
SVM Linear Grid – Species identification without film								
	Reference							
Prediction	*G.macrocefaphalus*	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
G.macrocefaphalus	11	0	0	0	0	0	0	0

G.morhua	0	0	0	0	0	0	1	0
L.piscatorius	0	0	4	0	0	0	0	0
L.vomerinus	0	0	0	3	0	0	0	0
O.nerka	0	0	0	0	0	0	0	0
P.virens	0	0	0	0	0	9	1	0
S.officinalis	1	1	2	0	0	0	15	0
S.salar	0	0	0	0	0	0	0	14

Supplementary Table 2b. Support vector machine confusion matrix results with and without film investigating status using the hold-out (70-30%) and an internal cross-validation.

SVM Radial Kernel – fresh or frozen and thawed status with film		
	Reference	
Prediction	FRESH	THAWED
FRESH	32	4
THAWED	6	23
SVM Radial Kernel – fresh or frozen-thawed status without film		
	Reference	
Prediction	FRESH	THAWED
FRESH	33	11
THAWED	5	16

Supplementary Table 3a. Support vector machine results for both datasets, with and without film, representing species identification tested using the hold-out (70-30%) and an internal cross-validation.

SVM Linear – Species identification with film								
	G.macrocefaphalus	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
Sensitivity	0.92	0	0.83	0.67	NA	0.78	0.88	1.00
Specificity	0.96	0.98	1.00	1.00	1.00	0.98	0.93	0.98
Pos Pred Value	0.85	0.00	1.00	1.00	NA	0.88	0.83	0.93
Neg Pred Value	0.98	0.98	0.98	0.98	NA	0.96	0.96	1.00
Prevalence	0.19	0.02	0.10	0.05	0.00	0.15	0.27	0.23
Detection Rate	0.18	0.00	0.08	0.03	0.00	0.11	0.24	0.23
Detection Prevalence	0.21	0.02	0.08	0.03	0.00	0.13	0.29	0.24
Balanced Accuracy	0.94	0.49	0.92	0.83	NA	0.88	0.91	0.99
SVM Linear Grid – Species identification with film								
	G.macrocefaphalus	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
Sensitivity	0.92	1.00	0.50	0.67	NA	0.89	0.88	1.00
Specificity	0.94	0.98	0.98	1.00	1.00	0.98	0.98	0.98
Pos Pred Value	0.79	0.50	0.75	1.00	NA	0.89	0.94	0.93
Neg Pred Value	0.98	1.00	0.95	0.98	NA	0.98	0.96	1.00
Prevalence	0.19	0.02	0.10	0.05	0.00	0.15	0.27	0.23
Detection Rate	0.18	0.02	0.05	0.03	0.00	0.13	0.24	0.23
Detection Prevalence	0.23	0.03	0.07	0.03	0.00	0.15	0.26	0.24
Balanced Accuracy	0.93	0.99	0.74	0.83	NA	0.94	0.93	0.99
SVM Linear – Species identification without film								
	G.macrocefaphalus	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
Sensitivity	0.92	0.00	0.50	1.00	NA	1.00	0.88	1.00
Specificity	0.96	0.98	1.00	1.00	1.00	1.00	0.91	1.00
Pos Pred Value	0.85	0.00	1.00	1.00	NA	1.00	0.79	1.00
Neg Pred Value	0.98	0.98	0.95	1.00	NA	1.00	0.95	1.00
Prevalence	0.19	0.02	0.10	0.05	0.00	0.15	0.27	0.23
Detection Rate	0.18	0.00	0.05	0.05	0.00	0.15	0.24	0.23
Detection Prevalence	0.21	0.02	0.05	0.05	0.00	0.15	0.31	0.23
Balanced Accuracy	0.94	0.49	0.75	1.00	NA	1.00	0.90	1.00
SVM Linear Grid – Species identification without film								
	G.macrocefaphalus	*G.morhua*	*L.piscatorius*	*L.vomerinus*	*O.nerka*	*P.virens*	*S.officinalis*	*S.salar*
Sensitivity	0.92	0.00	0.67	1.00	NA	1.000	0.88	1.00
Specificity	1.00	0.98	1.00	1.00	1.0 0	0.98	0.91	1.00
Pos Pred Value	1.00	0.00	1.00	1.00	NA	0.90	0.79	1.00
Neg Pred Value	0.98	0.98	0.97	1.00	NA	1.00	0.95	1.00
Prevalence	0.19	0.02	0.10	0.05	0.00	0.15	0.27	0.23

Detection Rate	0.18	0.00	0.07	0.05	0.00	0.15	0.24	0.23
Detection Prevalence	0.18	0.02	0.07	0.05	0.00	0.16	0.31	0.23
Balanced Accuracy	0.96	0.49	0.83	1.00	NA	0.99	0.90	1.00

* NA, not available. Due to the data absence, the performance metric cannot be calculated for the test set.

Supplementary Table 3b. Support vector machine results for both datasets, with and without film, representing status identification tested using the hold-out (70-30%) and an internal cross-validation.

SVM Radial Kernel – fresh or frozen-thawed status with film	
Sensitivity	0.84
Specificity	0.85
Pos Pred Value	0.89
Neg Pred Value	0.79
Prevalence	0.59
Detection Rate	0.49
Detection Prevalence	0.55
Balanced Accuracy	0.85
SVM Radial Kernel – fresh or frozen-thawed status without film	
Sensitivity	0.87
Specificity	0.59
Pos Pred Value	0.75
Neg Pred Value	0.76
Prevalence	0.59
Detection Rate	0.51
Detection Prevalence	0.68
Balanced Accuracy	0.73