Aquaphotomics and NIR Water Spectral Patterns in Dairy Production: Exploring Potentials and Challenges - A Review

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SUPPLEMENTARY FILE

Supplementary Table S1: World cow's milk production (tons x 1000) from 2012 to 2020. Modified version from CLAL, 2023

CONTINENT	2013	2014	2015	2016	2017	2018	2019	2020	2021
ASIA	176.075	185.199	191.248	196.307	205.518	214.903	224.998	242.774	246.092
EUROPE	211.904	218.132	221.233	220.98	223.296	225.817	227.265	229.97	226.645
AMERICA	180.089	183.523	185.628	184.996	187.594	190.395	191.481	196.341	197.644
AFRICA	37.275	37.399	37.316	37.995	38.291	38.926	40.701	42.65	42.509
OCEANIA	29.014	30.889	31.45	30.88	30.499	31.258	30.601	30.69	30.765
TOTAL	**634.357**	**655.142**	**666.875**	**671.158**	**685.198**	**701.299**	**715.046**	**742.425**	**743.655**
% INCREASE REFERRED TO THE PREVIOUS YEAR		*+3.28%*	*+1.79%*	*+0.64%*	*+2.09%*	*+2.35%*	*+1.96%*	*+3.83%*	*+0.14%*

Supplementary Table S2: List of publications resulting from the survey with Scopus Database and Google Scholar (up to June 2023) organised according to the thematic categories of the references. Section a reports references referred to "Fundamental of aquaphotomics", "Studies on water solutions", and "Food Quality"; Table 2b reports references referred to "Plant Biology and Agriculture", "Microbiology and Process Quality" and "Materials and nanomaterials"; Table 2c reports references referred to "Human Medicine" and "Veterinary Medicine".

	Thematic	Fundamentals of aquaphotomics	Studies on water solutions	Food Quality
2a	**Objectives**	Studies aimed at highlighting the molecular role of water in a system and the information potentially resulting from the interaction between NIR and matter. Definition of methods, objectives and introduction of the first results with a description of potential applications in scientific research as well as in practice.	Research activities involve monitoring changes in the spectral model of water as a function of any environmental perturbation, such as a change in temperature or the sample's composition.	Articles that use aquaphotomics as a tool to guarantee the safety and compliance of the product with the reference legislation, to protect the health of the consumer, to allow the detection of food fraud or the determination of the nutritional properties of food and beverages.
	References	Tsenkova, (2009); Tsenkova, (2010); Cattaneo *et al.* (2015a); Tsenkova *et al.* (2015); Kojić *et al.* (2017); Tsenkova *et al.* (2018); Muncan & Tsenkova (2019a); Van de Kraats *et al.* (2019); Cui, (2022); Roger *et al.* (2022); Ye *et al.* (2022); Ma *et al.* (2023); Muncan & Tsenkova (2023a)	Tsenkova, (2007b); Tsenkova, (2008b); Vero *et al.* (2010); Gowen *et al.* (2011a); Gowen *et al.* (2011b); Meilina *et al.* (2011); Muncan & Janjic (2012); Gowen *et al.* (2013); Muncan & Koruga (2013); Bazar *et al.* (2014); Bazar *et al.* (2015); Gowen *et al.* (2015); Kovacs *et al.* (2015); Cui *et al.* (2016); Putra *et al.* (2016); Cui *et al.* (2017); Kaur *et al.* (2017); Putra *et al.* (2017); Cui *et al.* (2018); Cui *et al.* (2019a); Dong *et al.* (2019a); Dong *et al.* (2019b); Li *et al.* (2019); Kovacs *et al.* (2020); Renati *et al.* (2020); Bozhynov *et al.* (2021); Dong *et al.* (2022); Han *et al.* (2022); Kovacs *et al.* (2022); Stoilov *et al.* (2022); Zhang *et al.* (2023a); Zhang *et al.* (2023b)	Esquerre *et al.* (2009a); Esquerre *et al.* (2009b); Gowen *et al.* (2009); Williams, (2009); Omar *et al.* (2012); Barzaghi *et al.* (2014); Muncan *et al.* (2014); Atanassova, (2015); Bazar *et al.* (2016); Cattaneo *et al.* (2016); Barzaghi *et al.* (2017); Veleva-Doneva, (2017a); Veleva-Doneva, (2017b); Vanoli *et al.* (2018); Sannia *et al.* (2019); Vanoli *et al.* (2019); Vitalis *et al.* (2019); Zaukuu *et al.* (2019); Brambilla *et al.* (2020); Kamboj *et al.* (2020); Kaur *et al.* (2020); Yang *et al.* (2020); Cattaneo *et al.* (2021); Kato *et al.* (2021); Muncan *et al.* (2021b); Nagy *et al.* (2021); Aouadi *et al.* (2022); Bodor *et al.* (2022); Cattaneo *et al.* (2022a); Kaur *et al.* (2022a); Kaur *et al.* (2022b); Malegori *et al.* (2022); Marinoni *et al.* (2022a); Marinoni *et al.* (2022b); Muncan *et al.* (2022c); Rajkumar *et al.* (2022); Raypah *et al.* (2022a); Su *et al.* (2022); Atanassova *et al.* (2023); Vitalis *et al.* (2023)

	Thematic	Plant Biology and Agriculture	Microbiology and Process Quality	Materials and nanomaterials
2b	**Objectives**	It is possible to detect changes at a molecular level in a plant subjected to biotic or abiotic stress or during the succession of the different phases of its biological life cycle. This scientific discipline also applies to evaluating and analysing water in an aquaponic system as a guarantee of productivity and growth efficiency of cultivated plant species.	Instrumental control of the growth of bacterial strains such as to allow their better characterisation and targeted selection for the optimisation of industrial processes. Research activities for monitoring the efficiency of treatment and the performance of an industrial manufacturing process.	Studies aim to understand the chemical, physical and biological properties of fundamental materials such as those used in the biomedical field.
	References	Jinendra *et al.* (2010); Cattaneo *et al.* (2015b); Bozhynov *et al.* (2018); Kuroki *et al.* (2019); Muncan *et al.* (2019b); Muncan *et al.* (2019c); Mura *et al.* (2019); Concepcion *et al.* (2020); Lauguico *et al.* (2020); Muncan *et al.* (2020b); Alajas *et al.* (2021); Concepcion *et al.* (2021); Kovacs *et al.* (2021); Nugraha *et al.* (2021); Bruñas Gómez *et al.* (2022); Cattaneo *et al.* (2022b); Concepcion *et al.* (2022); Muncan *et al.* (2022a); Zahir *et al.* (2022)	Remagni *et al.* (2013); Slavchev *et al.* (2015); Slavchev *et al.* (2017); Kovacs *et al.* (2019); Nath *et al.* (2021) Thierie, (2012); Muncan *et al.* (2020a); Gao *et al.* (2021); Muncan *et al.* (2021a); Gao *et al.* (2022)	Matija *et al.* (2012); Matija *et al.* (2013); Tomic *et al.* (2013); Tomic *et al.* (2014); Muncan *et al.* (2016); Sakota Rosic *et al.* (2016); Matija *et al.* (2017); Muncan, (2017); Dong *et al.* (2020); Tian *et al.* (2021); Muncan *et al.* (2022b); Wei *et al.* (2022); Gao *et al.* (2023); Tian *et al.* (2023)

	Thematic	Human medicine	Veterinary medicine
2c	**Objectives**	Studies use water as a biomarker for the early and non-invasive diagnosis of disease before the clinical manifestation of symptoms, as well as a sensor for monitoring the effects of therapy on the body at the molecular level.	Aquaphotomics application foresee the use of water as an essential source of information for diagnostic applications and timely health treatment, reducing economic and production losses for the farm.
	References	Chatani *et al.* (2014); Goto *et al.* (2015); Zunjic *et al.* (2015); Cui *et al.* (2019b); Baishya *et al.* (2020); Li *et al.* (2020); Baishya *et al.* (2021); Liu *et al.* (2021); Zhang *et al.* (2021); Raypah *et al.* (2022b); Raypah *et al.* (2022c); Scholkmann & Tsenkova (2022)	Tsenkova, (2006); Tsenkova, (2007a); Tsenkova, (2008a); Kinoshita *et al.* (2012); Kinoshita *et al.* (2015); Takemura *et al.* (2015); Agcanas *et al.* (2017); Counsell *et al.* (2017); Vance *et al.* (2017); Santos-Rivera *et al.* (2021); Tsenkova & Muncan (2021); Santos-Rivera *et al.* (2022a); Santos-Rivera *et al.* (2022b); Santos Rivera & Mariana (2022c); Muncan *et al.* (2023b)

FIGURE LEGENDS:

Supplementary Figure S1: Distribution of articles focused on the theme of Aquaphotomics classified according to the year of publication.

Supplementary Figure S2: Transformed NIR spectra (A), Aquagram (B) and PCA-LDA (C) plot from bovine blood plasma collected before and after microorganism infection (Santos-Rivera et al. 2021).

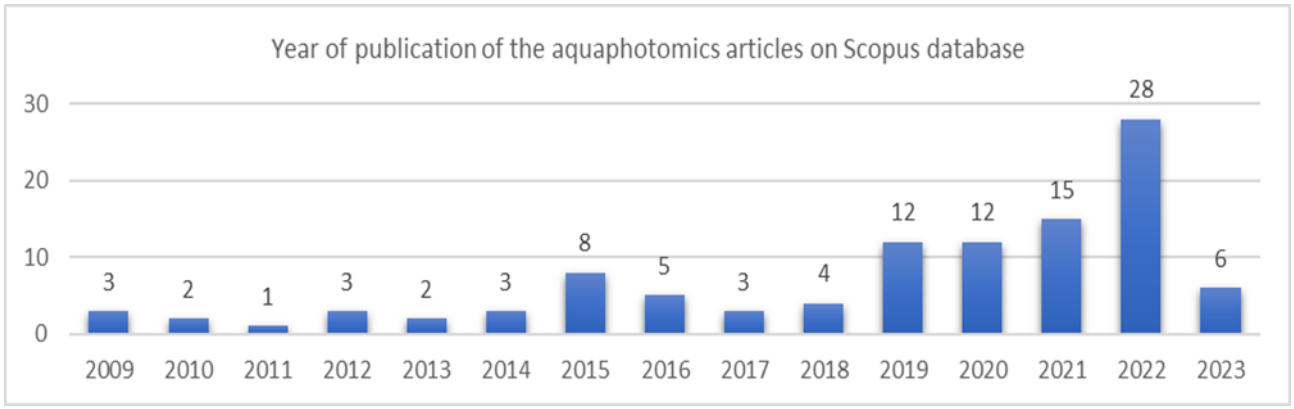
Supplementary Figure S3: PCA (A) and Aquagram (B) of healthy, pre-diabetes, and type 2 diabetes samples (Li et al. 2020).

Supplementary Figure S4: Aquagram of lactose solutions at different concentrations (Bazar et al. 2015).

Supplementary Figure S5: NIR water spectral pattern of cheese samples with different food coating materials (Cattaneo et al. 2016).

742 **FIGURES**

743 **Supplementary Figure S1:**



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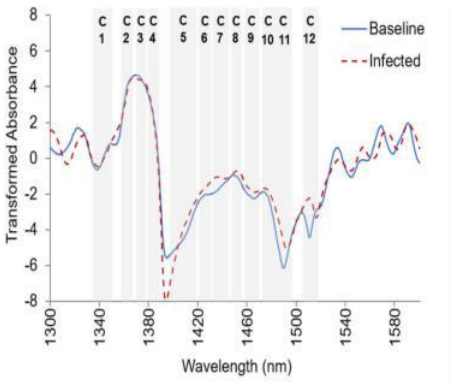
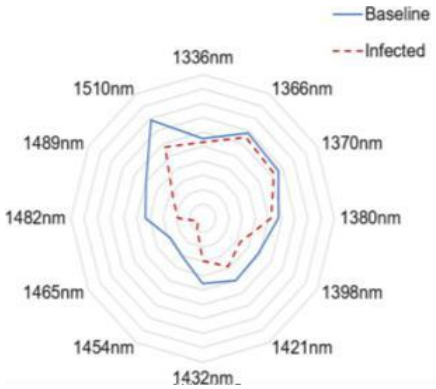
746 **Supplementary Figure S2:**



A



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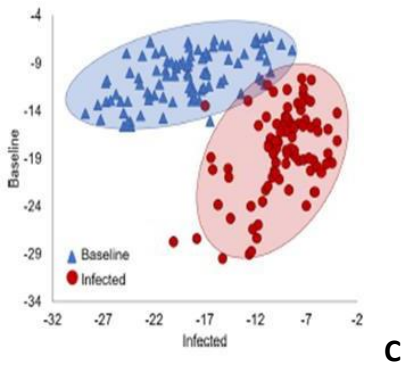

748 **C**

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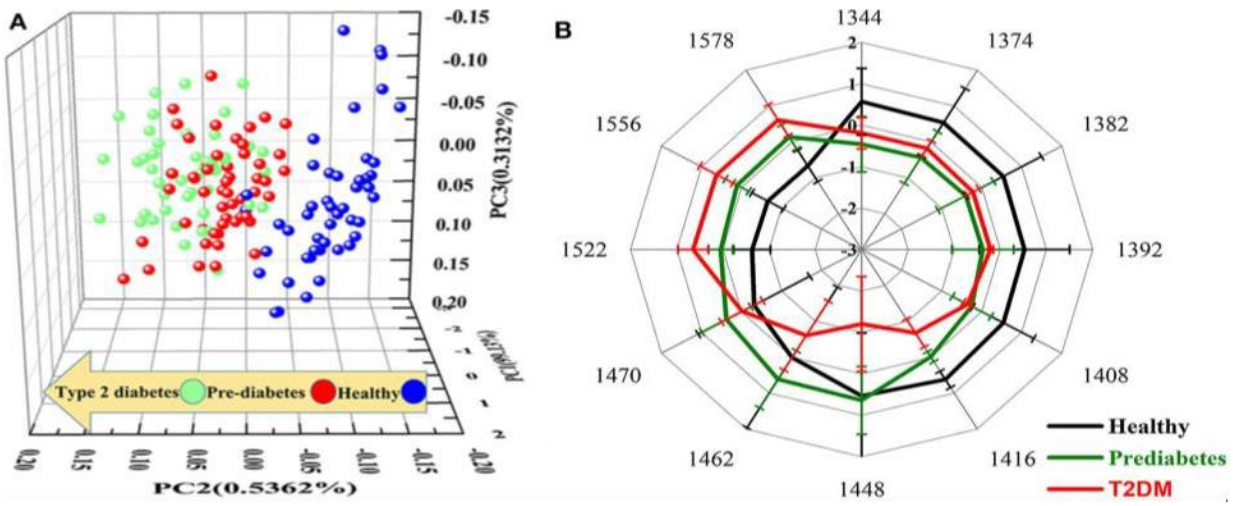
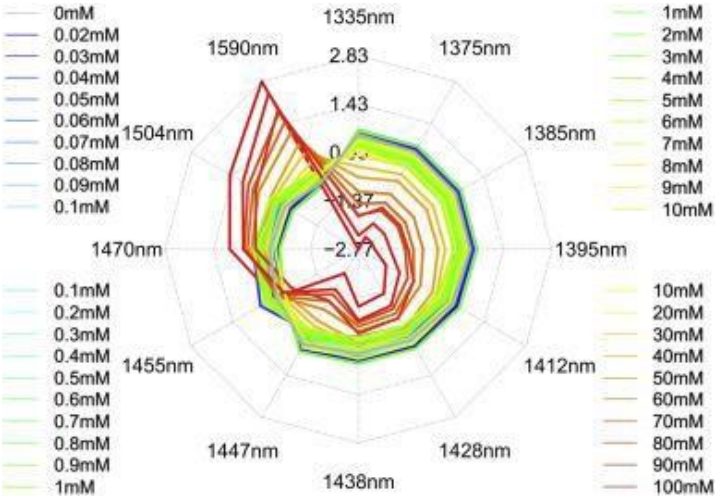
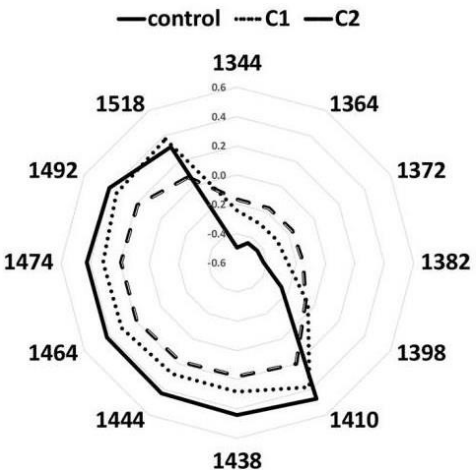
Supplementary Figure S3:



Supplementary Figure S4:



Supplementary Figure S5:



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