Supplementary Material

# Supplementary Data

Table S1. The absorbance bands that showed importance for storage monitoring and/or discrimination between the type of cold storage of strawberries, and their positions within the previously discovered water matrix coordinate (WAMACS) ranges (1), with tentative proposal for 4 new WAMACS

|  |  |  |
| --- | --- | --- |
| Absorbance band (nm) | Source (analysis) | WAMACS (1–3) |
| 1311 | SIMCA results for CF group (Fig.3a) |  |
| 1311 | SIMCA results for SCF group (Fig.3b) |  |
| 1323 | SIMCA results for CF group (Fig.3a) |  |
| 1329 | PLSR model for 15 days storage period (Fig.4d) |  |
| **1348** | The difference spectra of SCF during the storage (Fig.2d) | **C1** (1336-1348 nm) |
| **1348** | PLSR model for 15 days storage period (Fig.4d) |
| 1350 | PLSR model for 4 days storage period (Fig.4c) |  |
| **1360** | SIMCA results for CF group (Fig.3a) | **C2** (1360-1366 nm) |
| **1360** | SIMCA results for SCF group (Fig.3b) |
| **1360** | PLSR model for 15 days storage period (Fig.4d) |
| **1373** | The difference spectra of CF during the storage (Fig.2c) | **C3** (1370-1376 nm) |
| **1373** | The difference spectra of SCF during the storage (Fig.2d) |
| **1373** | PLSR model for 4 days storage period (Fig.4c) |
| **1379** | SIMCA results for CF group (Fig.3a) | **C4** (1380-1388 nm) |
| **1379** | SIMCA results for SCF group (Fig. 3b) |
| **1379** | PLSR model for 4 days storage period (Fig.4c) |
| **1379** | PLSR model for 15 days storage period (Fig.4d) |
| **1385** | The difference spectra before storage and after 1 day of storage (Fig.2a) |
| **1385** | The difference spectra before and after 4 days of storage (Fig.2b) |
| **1385** | The difference spectra of CF during the storage (Fig.2c) |
| **1385** | PLSR model for 4 days storage period (Fig.4c) |
| **1391** | The difference spectra of SCF during the storage (Fig.2d) | **C5** (1396-1403 nm) |
| **1391** | PLSR model for 4 days storage period (Fig.4c) |
| **1391** | PLSR model for 15 days storage period (Fig.4d) |
| **1397** | PLSR model for 15 days storage period (Fig.4d) |
| **1404** | The difference spectra before storage and after 1 day of storage (Fig.2a) | **C5** (1404-1414 nm) |
| **1404** | PLSR model for 15 days storage period (Fig.4d) |
| **1410** | The difference spectra before and after 4 days of storage (Fig.2b) |
| **1410** | The difference spectra of CF during the storage (Fig.2c) |
| **1410** | PLSR model for 4 days storage period (Fig.4c) |
| **1416** | PLSR model for 4 days storage period (Fig.4c) |
| **1428** | The difference spectra before and after 4 days of storage (Fig.2b) | **C6** (1421-1430 nm) |
| **1428** | PLSR model for 4 days storage period (Fig.4c) |
| **1428** | PLSR model for 15 days storage period (Fig.4d) |
| **1435** | PLSR model for 4 days storage period (Fig.4c) | **C7** (1432-1444 nm) |
| **1441** | PLSR model for 15 days storage period (Fig.4d) |
| **1447** | The difference spectra before and after 4 days of storage (Fig.2b) | **C8** (1448-1454 nm) |
| **1447** | The difference spectra of SCF during the storage (Fig.2d) |
| **1447** | SIMCA results for CF group (Fig. 3a) |
| **1447** | SIMCA results for SCF group (Fig. 3b) |
| **1447** | PLSR model for 4 days storage period (Fig.4c) |
| **1453** | SIMCA results for CF group (Fig. 3a) |
| **1453** | PLSR model for 15 days storage period (Fig.4d) |
| **1459** | The difference spectra of CF during the storage (Fig.2c) | **C9** (1458-1468 nm) |
| **1459** | The difference spectra of SCF during the storage (Fig.2d) |
| **1459** | PLSR model for 4 days storage period (Fig.4c) |
| **1466** | PLSR model for 15 days storage period (Fig.4d) |
| **1472** | PLSR model for 15 days storage period (Fig.4d) | **C10** (1472-1482 nm) |
| **1478** | The difference spectra of CF during the storage (Fig.2c) |
| **1478** | The difference spectra of SCF during the storage (Fig.2d) |
| **1478** | PLSR model for 4 days storage period (Fig.4c) |
| **1478** | PLSR model for 15 days storage period (Fig.4d) |
| **1484** | SIMCA results for CF group (Fig.3a) | **C11** (1482-1495 nm) |
| **1484** | PLSR model for 15 days storage period (Fig.4d) |
| **1490** | The difference spectra of SCF during the storage (Fig.2d) |
| **1490** | PLSR model for 4 days storage period (Fig.4c) |
| **1497** | SIMCA results for CF group (Fig.3a) |
| **1497** | PLSR model for 15 days storage period (Fig.4d) |
| **1503** | The difference spectra of CF during the storage (Fig.2c) | **Ci** |
| **1503** | The difference spectra of SCF during the storage (Fig.2d) |
| **1503** | SIMCA results for SCF group (Fig. 3b) |
| **1503** | PLSR model for 15 days storage period (Fig.4d) |
| 1509 | SIMCA results for CF group (Fig. 3a) | **C12** (1506-1516 nm) |
| 1521 | PLSR model for 15 days storage period (Fig.4d) |
| **1528** | SIMCA results for CF group (Fig.3a) | **Cj** |
| **1528** | SIMCA results for SCF group (Fig.3b) |
| **1528** | PLSR model for 4 days storage period (Fig.4c) |
| **1528** | PLSR model for 15 days storage period (Fig.4d) |
| **1534** | The difference spectra of CF during the storage (Fig.2c) | **Ck** |
| **1534** | The difference spectra of SCF during the storage (Fig.2d) |
| **1534** | SIMCA results for CF group (Fig.3a) |
| **1534** | SIMCA results for SCF group (Fig.3b) |
| **1534** | PLSR model for 15 days storage period (Fig.4d) |
| 1540 | PLSR model for 15 days storage period (Fig.4d) |  |
| 1550 | PLSR model for 15 days storage period (Fig.4d) |  |
| **1559** | SIMCA results for CF group (Fig.3a) | **Cl** |
| **1559** | SIMCA results for SCF group (Fig. 3b) |
| **1559** | PLSR model for 4 days storage period (Fig.4c) |
| **1559** | PLSR model for 15 days storage period (Fig.4d) |
| 1571 | PLSR model for 15 days storage period (Fig.4d) |  |
| 1577 | PLSR model for 15 days storage period (Fig.4d) |  |
| 1583 | PLSR model for 15 days storage period (Fig.4d) |  |

Table S2. Tentative proposal of four new WAMACS with their assignment and information about the related functionality in aqueous and biological systems

|  |  |
| --- | --- |
| Absorbance band (nm) | Potential assignment / Functionality |
| 1503 | 1503 nm – strongly bound water, influential variable in modeling of ascorbic acid content in mung bean (in living matrixes, AA has tendency to create efficient inter-molecular hydrogen bonds)(4)  1503 nm – influential variable in prediction of water content in human nails (5)  1503 nm – important variable for early diagnosis of cassava frog skin disease in powdered tissue samples (6)  1503 nm – water absorption wavelength, reflects moisture content in maize leaves (7)  1503 nm - important variable for detection of common scab skin disease of the potato tubers (8)  1503 nm (3326 cm-1) – strong intermolecular hydrogen bond in phenols (9)  1503 nm (3326 cm-1) – hydrogen bonded, NH stretching vibration in aqueous vinyl polymer solution (10)  1503 nm (3326 cm-1) - hydrogen-bonded N–H stretching mode (11)  1503 nm (3326 cm-1) – OH stretching vibrations of hydrogen bonded water molecules participating in the crystal structure (12)  1503 nm (3326 cm-1) – water stretching vibrations in minerals, in connection with defects (13–15)  1503 nm (3326 cm-1) – OH stretching vibration in Ice III (16)  1503 nm (3326 cm-1) – H-related defects gives rise to O-H local vibrational mode absorption at 3326 and 3611 cm-1(17)  1503 nm (3326 cm−1) - attributed to OH group located in a vacant site; vibrational mode of hydrous defect in wadsleyite mineral; related to incorporation of hydrogen (protonation) (18)  1503 nm (3326 cm−1) – hydroxyl group in raw starch material, affected by glutaraldehyde vapor phase crosslinking; becomes wider and weaker (19)  1503 nm (3326 cm−1) – OH stretching line assigned to a shallow donor that is introduced by H into ZnO crystals(20)  1503 nm (3326 cm−1) – hydrogen defect in ZnO (21)  1503 (3326 cm−1 ) – hydrogen bond on O site, in relation to protonation of O on anomalous oxygen site (22) |
| 1528 | 1528 nm – starch OH stretch, hydrogen bonded intramolecular or intermolecular with water molecules; associated with differences in level of mechanical damage (23) |
| 1534 | 1534 nm – one of 3 wavelengths used in multiple linear regression for predicting bread loaf volume (1506, 1534 and 1618 nm); measurement of some parameter related to volume independent of protein (24)  1534 nm – 1st overtone of NH stretching (25)  1534 (3259 cm-1) – N-H stretching (26,27)  1534 nm – one of 4 wavelengths (662, 686, 1534 and 1753 nm) used for improved prediction of chlorophyll content in intact canola (28)  1534 nm (3259 cm-1) – hydrogen bonded hydroxyl groups (–O–Hδ+···Oδ−–) (29)  1534 nm (3259 cm-1) the H–O stretching vibrations of the absorbent water (30)  1534 nm (6518 cm-1) – 1st over. of hydrogen bonded O-H stretching (31)  1534 (3259 cm-1) – one of the 3 water stretching bands observed in carbonate mineral huanghoite by Raman spectroscopy (the other two being 1435 nm (3484 cm-1) and 1393 nm (3589 cm-1)) (13)  1534 (3259 cm-1) – sesquihydrate crystallite (32) (hydrate whose solid contains 3 molecules of water of crystallization per two molecules)  1534 (3259 cm-1) – one of the vibrational frequencies that can be assigned to water heptamer (H2O)7 single H-donor OH stretch (33) |
| 1559 | 1560 nm – first overtone of glucose (34)  1560 nm – glucose band (35)  1559 nm (3207 cm-1)-OH group in D-(+)galactose (36)  1560 nm (6410 cm−1) - first overtone of the NH bond (calibration model for concentration of amino acid theanine in tea, indicator of fermentation) (37)  1559 nm – protein band in model for estimating soybean meal content in compound feeds (38)  1560 nm (6410 cm-1) -Amine b, Overtone of primary NH2 plus secondary NH stretching (39)  1560–1570 nm region- associations with starch and sugar, due to stretching O–H bonds, bands important for classification of vegetative growth stage in snapbean (40)  1560 nm – hydrogen bonded water, influenced by temperature in model membranes (41)  1560 nm (6410 cm-1) crystalline water ice feature (42)  1560 nm (6410 cm-1) – intensity decrease is an indicator of crystallinity decrease for a model polymorphic drug (43)  1560 nm (3205 cm-1)- strongly hydrogen-bonded water species (44)  1560 nm (3205 cm-1)-hydrogen bonded water to the chains of super absorbent polymer network chains (dewatering coal) (45)  1560 nm (3205 cm-1)-vibrations of the hydrogen-bonded water OH groups forming the ring structure (in naphtol-water clusters 1-naphtol·(H2O)3) (46)  1560 nm (3205 cm-1)-stretching of adsorbed water in pollen grains increasing with increased relative humidity (47)  1560 nm (3205 cm-1)-H-bonded O-H stretch (48,49)  1560 nm (3205 cm-1)- water pentamer (50)  1559 nm (3207 cm-1)-intramolecular hydrogen bonding from -OH···N or from OH···O (51)  1560 nm (3205 cm-1)-O-H asymmetric stretch in Zundel cation H5O2+(52)  1560 nm (3205 cm-1)-cyclic multimer (53)  1560 nm (3205 cm-1)-OH mode of strongly bounded adsorbed water molecules in cellulose (54,55)  1560 nm (3205 cm-1)- strongly hydrogen bonded water, water coordinated to cations (56) |

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