**Table S1.** Correlation matrix between all individual and groups of anthocyanins. Pearson correlation coefficients (r) are presented below the diagonal while the significance p-values are shown above the diagonal.

Total Anthocyanins (Total Anth.); Total 3-*O*-glucoside anthocyanins (Total Gl Anth.); Total 3-*O*-(6-acetyl)glucoside anthocyanins (Total GlAc Anth.); Total 3-*O*-(6-*p*-coumaroyl)glucoside anthocyanins (Total GlCm Anth.); Malvidin 3-*O*-glucoside (MvGl); Malvidin 3-*O*-(6-acetyl)glucoside (MvGlAc); Malvidin 3-*O*-(6-*p*-coumaroyl)glucoside (MvGlCm); Petunidin 3-*O*-glucoside (PtGl); Petunidin 3-*O*-(6-acetyl)glucoside (PtGlAc); Petunidin 3-*O*-(6-*p*-coumaroyl)glucoside (PtGlCm); Delphinidin 3-*O*-glucoside (DpGl); Delphinidin 3-*O*-(6-acetyl)glucoside (DpGlAc); Delphinidin 3-*O*-(6-*p*-coumaroyl)glucoside (DpGlCm); Peonidin 3-*O*-glucoside (PnGl); Peonidin 3-*O*-(6-acetyl)glucoside (PnGlAc); Peonidin 3-*O*-(6-*p*-coumaroyl)glucoside (PnGlCm); Cyanidin 3-*O*-glucoside (CyGl); Cyanidin 3-*O*-(6-acetyl)glucoside (CyGlAc); Cyanidin 3-*O*-(6-*p*-coumaroyl)glucoside (CyGlCm).

| | MvGl | MvGlAc | MvGlCm | PtGl | PtGlAc | PtGlCm | DpGl | DpGlAc | DpGlCm | PnGl | PnGlAc | PnGlCm | CyGl | CyGlAc | CyGlCm | Total Anth. | Total Gl Anth. | Total GlAc Anth. | Total GlCm Anth. |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **MvGl** | | <0.001 | <0.001 | <0.001 | 0.130 | <0.001 | <0.001 | 0.269 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| **MvGlAc** | 0.685 | | <0.001 | <0.001 | 0.011 | <0.001 | <0.001 | 0.230 | <0.001 | 0.114 | <0.001 | <0.001 | 0.207 | 0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| **MvGlCm** | 0.400 | 0.439 | | 0.917 | <0.001 | <0.001 | 0.253 | 0.537 | <0.001 | 0.007 | 0.034 | <0.001 | <0.001 | 0.853 | <0.001 | 0.283 | 0.767 | <0.001 | <0.001 |
| **PtGl** | 0.837 | 0.640 | -0.011 | | 0.921 | <0.001 | 0.085 | <0.001 | <0.001 | <0.001 | 0.197 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | 0.003 | <0.001 |
| **PtGlAc** | 0.164 | 0.272 | 0.511 | -0.011 | | <0.001 | 0.085 | 0.106 | <0.001 | 0.001 | 0.108 | 0.181 | 0.002 | 0.782 | 0.015 | 0.971 | 0.721 | <0.001 | 0.002 |
| **PtGlCm** | 0.741 | 0.877 | 0.706 | 0.577 | 0.413 | | <0.001 | 0.208 | <0.001 | 0.415 | <0.001 | <0.001 | 0.993 | 0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| **DpGl** | 0.821 | 0.775 | 0.125 | 0.922 | 0.187 | 0.730 | | 0.480 | <0.001 | <0.001 | <0.001 | 0.095 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| **DpGlAc** | 0.120 | 0.131 | 0.068 | 0.187 | -0.176 | 0.137 | 0.077 | | 0.426 | 0.001 | 0.159 | 0.010 | 0.005 | 0.128 | 0.184 | 0.056 | 0.057 | 0.331 | 0.335 |
| **DpGlCm** | 0.760 | 0.920 | 0.534 | 0.680 | 0.370 | 0.968 | 0.844 | 0.087 | | 0.176 | <0.001 | <0.001 | 0.314 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| **PnGl** | 0.486 | 0.172 | -0.288 | 0.737 | -0.344 | 0.089 | 0.446 | 0.361 | 0.147 | | <0.001 | 0.464 | <0.001 | 0.004 | 0.050 | <0.001 | <0.001 | 0.669 | 0.111 |
| **PnGlAc** | 0.783 | 0.674 | 0.229 | 0.817 | 0.175 | 0.692 | 0.873 | 0.153 | 0.777 | 0.407 | | 0.138 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 | <0.001 |
| **PnGlCm** | 0.383 | 0.407 | 0.657 | 0.140 | 0.146 | 0.608 | 0.181 | 0.276 | 0.468 | 0.080 | 0.161 | | 0.107 | 0.942 | <0.001 | 0.025 | 0.098 | <0.001 | 0.001 |
| **CyGl** | 0.409 | 0.138 | -0.408 | 0.732 | -0.326 | 0.001 | 0.469 | 0.300 | 0.110 | 0.921 | 0.442 | -0.195 | | 0.001 | 0.268 | <0.001 | <0.001 | 0.104 | 0.173 |
| **CyGlAc** | 0.670 | 0.356 | -0.006 | 0.668 | 0.030 | 0.356 | 0.709 | 0.165 | 0.431 | 0.309 | 0.733 | -0.008 | 0.345 | | 0.004 | <0.001 | <0.001 | 0.210 | <0.001 |
| **CyGlCm** | 0.769 | 0.841 | 0.614 | 0.619 | 0.262 | 0.929 | 0.732 | 0.145 | 0.921 | 0.212 | 0.703 | 0.604 | 0.121 | 0.306 | | <0.001 | <0.001 | <0.001 | <0.001 |
| **Total Anth.** | 0.915 | 0.701 | 0.121 | 0.982 | 0.004 | 0.678 | 0.915 | 0.216 | 0.754 | 0.717 | 0.833 | 0.250 | 0.691 | 0.622 | 0.718 | | <0.001 | <0.001 | <0.001 |
| **Total Gl Anth.** | 0.890 | 0.649 | 0.034 | 0.989 | -0.041 | 0.608 | 0.903 | 0.214 | 0.698 | 0.756 | 0.822 | 0.186 | 0.741 | 0.633 | 0.657 | 0.996 | | 0.001 | <0.001 |
| **Total GlAc Anth.** | 0.716 | 0.993 | 0.445 | 0.668 | 0.335 | 0.894 | 0.797 | 0.109 | 0.935 | 0.180 | 0.704 | 0.376 | 0.154 | 0.384 | 0.840 | 0.708 | 0.654 | | 0.726 |
| **Total GlCm Anth.** | 0.619 | 0.709 | 0.906 | 0.327 | 0.396 | 0.916 | 0.452 | 0.110 | 0.808 | -0.048 | 0.470 | 0.736 | -0.183 | 0.142 | 0.851 | 0.448 | 0.362 | <0.001 | |

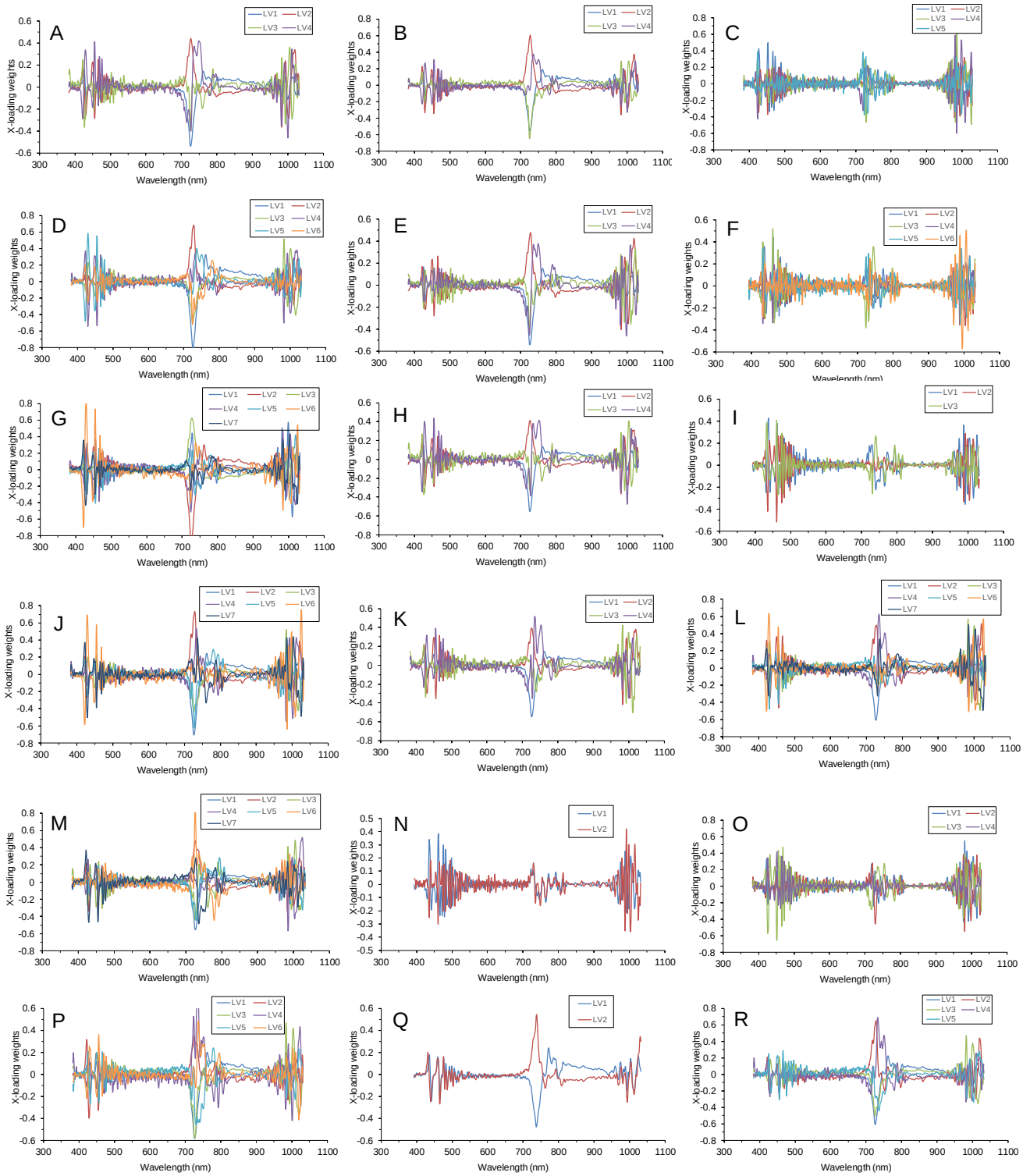


**Figure S1.** Loadings of the best MPLS calibration models reported in Table 3 for (A) Total anthocyanins; (B) Total 3-*O*-glucoside anthocyanins; (C) Total 3-*O*-(6-acetyl)glucoside anthocyanins; (D) Total 3-*O*-(6-*p*-coumaroyl)glucoside anthocyanins; (E) Malvidin 3-*O*-glucoside; (F) Malvidin 3-*O*-(6-acetyl)glucoside; (G) Malvidin 3-*O*-(6-*p*-coumaroyl)glucoside; (H) Petunidin 3-*O*-glucoside; (I) Petunidin 3-*O*-(6-acetyl)glucoside; (J) PtGlCm: Petunidin 3-*O*-(6-*p*-coumaroyl)glucoside; (K) DpGl: Delphinidin 3-*O*-glucoside; (L) Delphinidin 3-*O*-(6-*p*-coumaroyl)glucoside; (M) Peonidin 3-*O*-glucoside; (N) Peonidin 3-*O*-(6-acetyl)glucoside; (O) Peonidin 3-*O*-(6-*p*-coumaroyl)glucoside; (P) Cyanidin 3-*O*-glucoside; (Q) Cyanidin 3-*O*-(6-acetyl)glucoside; (R) Cyanidin 3-*O*-(6-*p*-coumaroyl)glucoside.