

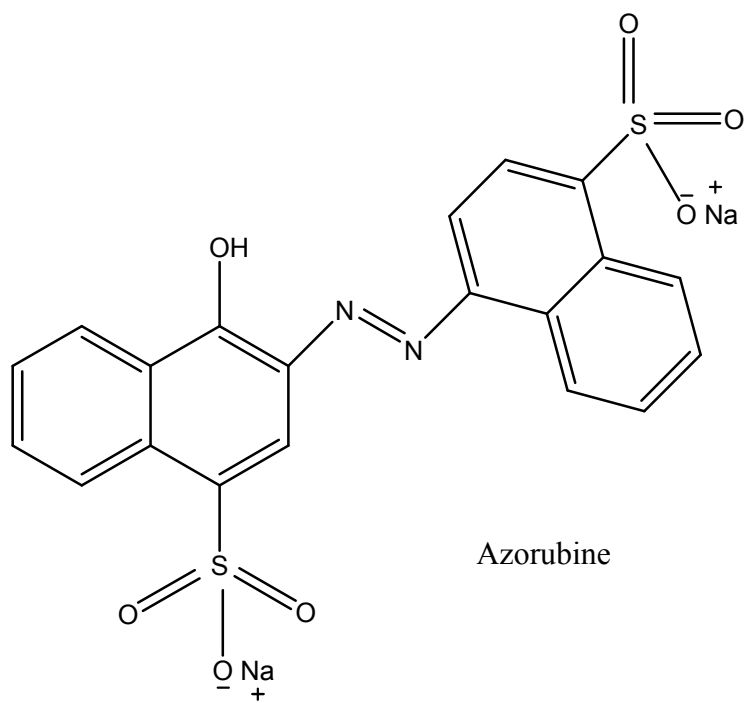
Table S1. Major IR absorption bands and possible assignment in the typical FT-IR spectrum of saffron

<i>Band (cm⁻¹)*</i>	<i>Assignment</i>
3365–3333 (broad)	Stretching vibration of bonded and non-bonded –O–H groups
2924 (m) and 2857 (m)	Asymmetric –CH ₂ –, symmetric –CH ₃ and –CH ₂ – stretching vibrations
1745–1696 (sh)	–C=O stretching vibrations (e.g. in the –COOR groups of crocetin/–COOH groups of aminoacids)
1659–1653 (s)	=C–H stretching vibrations (e.g. in the RCH=CHR' groups of crocetin)/amide I/O–H bending vibrations in water
1613 (m)	C–C skeletal vibrations
1580–1578 (m) and 1545–1542 (sh)	C–O vibrations (e.g. in the –COOR groups of crocetin)/amide II/aromatic –C=C stretching vibrations
1454 (w)	C–H bending (scissoring) (in CH ₃ groups)/aromatic –C=C stretching vibrations
1400 (w) and 1375 (w)	–OH bending vibrations, –C–O–H in-plane bending vibrations, –CH ₃ out-of-plane bending vibrations, –CH ₂ – wagging and twisting vibrations
1317 (w), 1294–1292 (w), 1271 (w) and 1227 (s)	C(O)–O stretching vibrations and –OH in plane vibrations/amide III (e.g. in aromatic ethers)
1157 (sh)	C–O stretching vibrations (e.g. in C–O–C glycosidic linkages of oligosaccharides or in triacylglycerols)
1075 (s)	C–1–H bending vibration in sugars
1020 (sh)	C–4–OH (typical for glucose residue of disaccharides)
970–920 (sh)	trans = C–H out-of-plane bending
780–700 (w)	cis = C–H out-of-plane bending

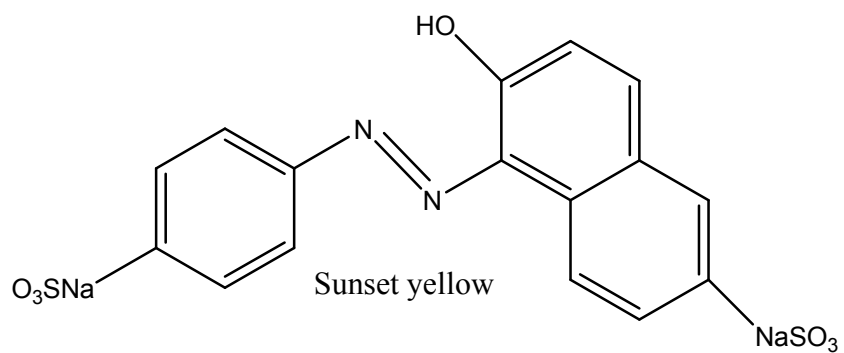
* m: medium; s: strong; sh: shoulder; w: weak.

Table S2. The results of PCA application on the transmittance FT-IR spectral data of Saffron samples

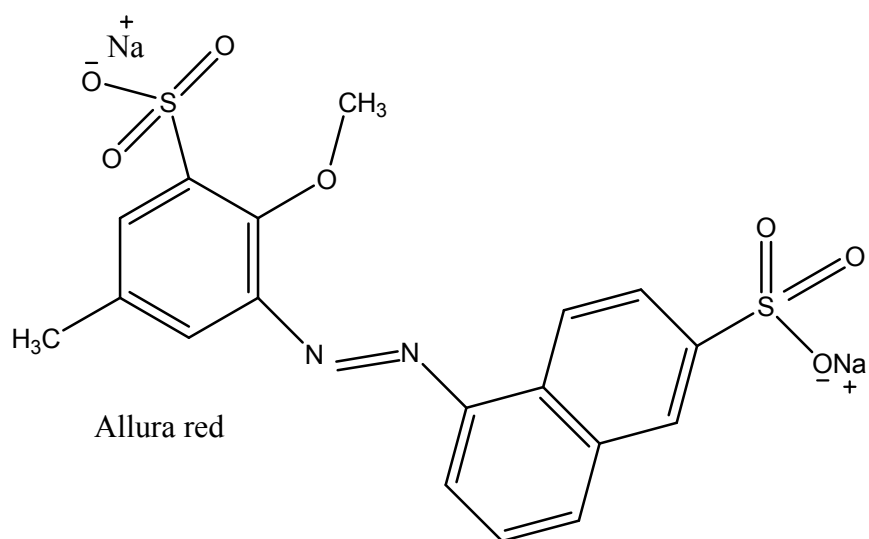
Component	Eigen-value	Percent of Variance	Cumulative percent of variances
1	14.5	77.80	77.80
2	3.20	17.13	94.92
3	1.06	2.69	97.61
4	0.23	0.83	98.45



Azorubine



Sunset yellow



Allura red

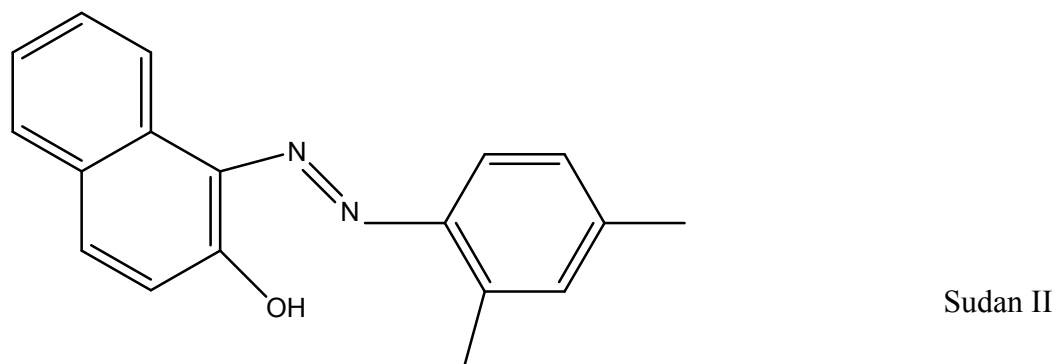
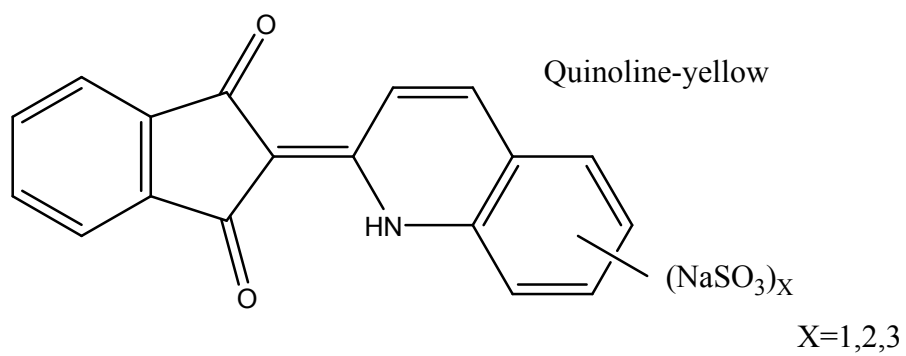
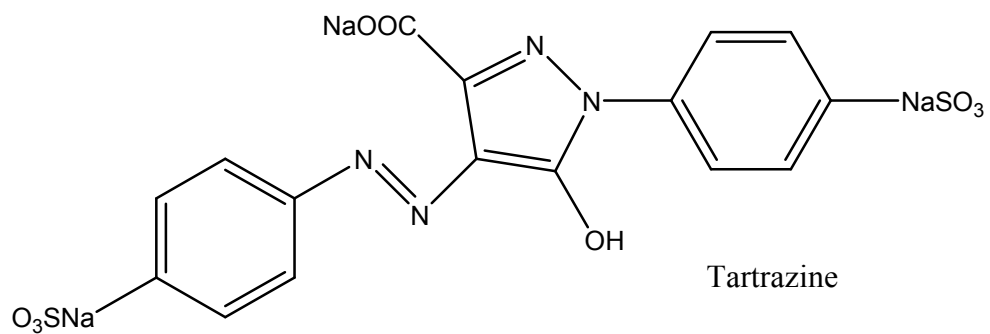


Figure (S1) .Chemical structure of food colorant

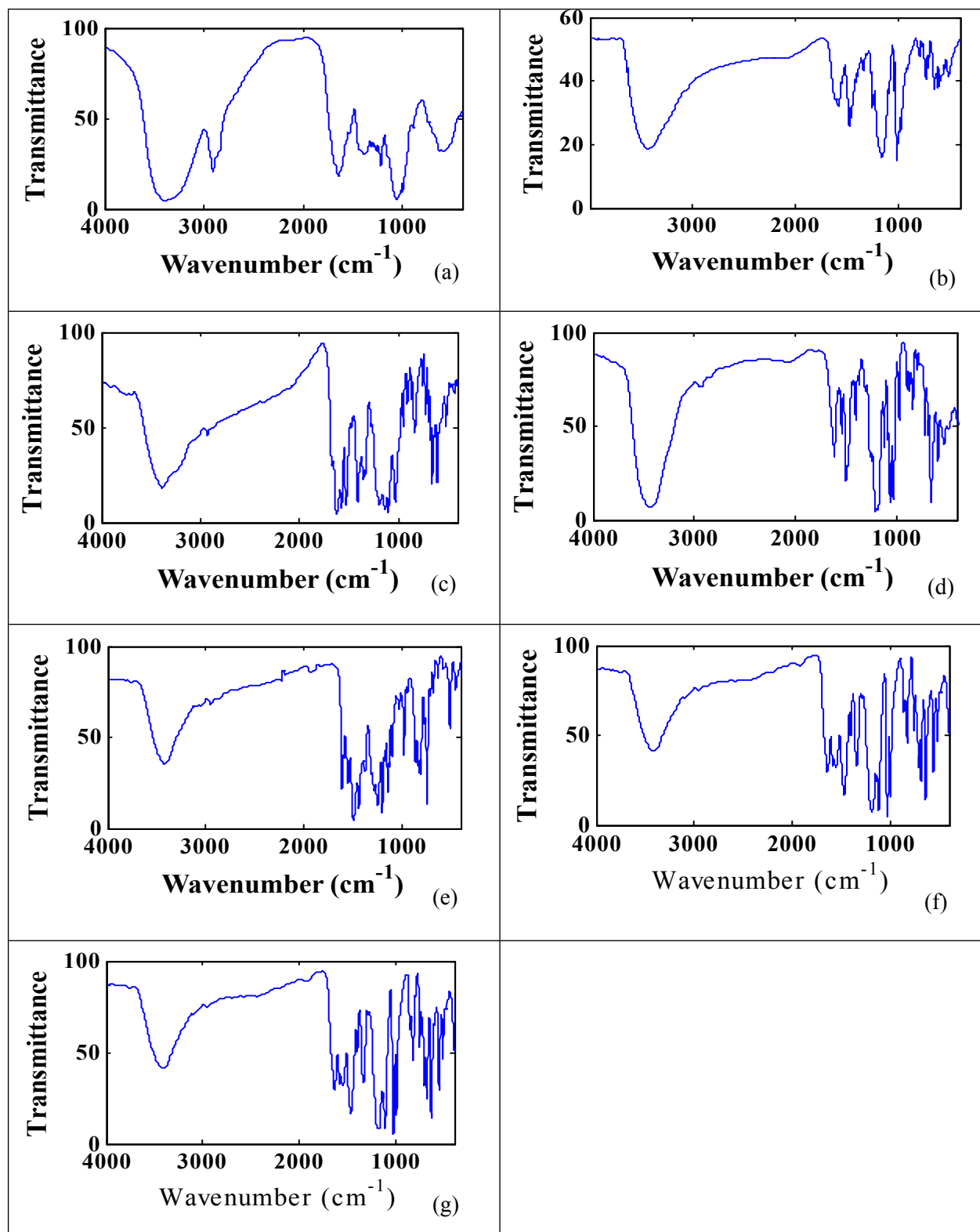


Figure (S2). (a) Saffron (b) Azorubine (c) Quinoline yellow (d) Allura red (e) Sudan (II) (f) Sunset yellow (g) Tartrazine

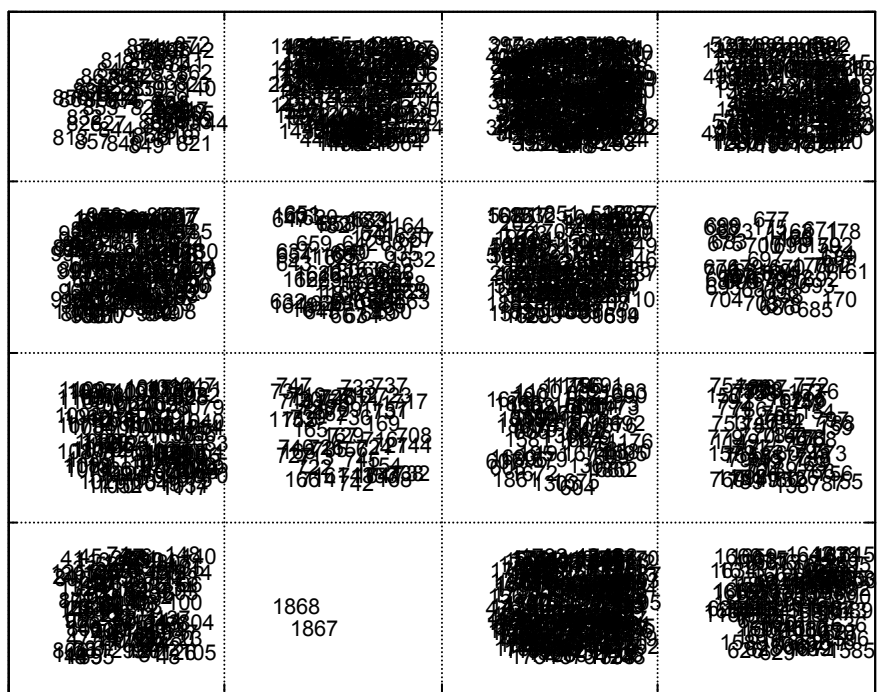


Figure S3. Distribution pattern of the wavenumbers from saffron data set obtained using 4-node Kohonen SOM for clustering of wavenumbers. The numbers from 1–1868 refer to the wavenumber transmittance data set.

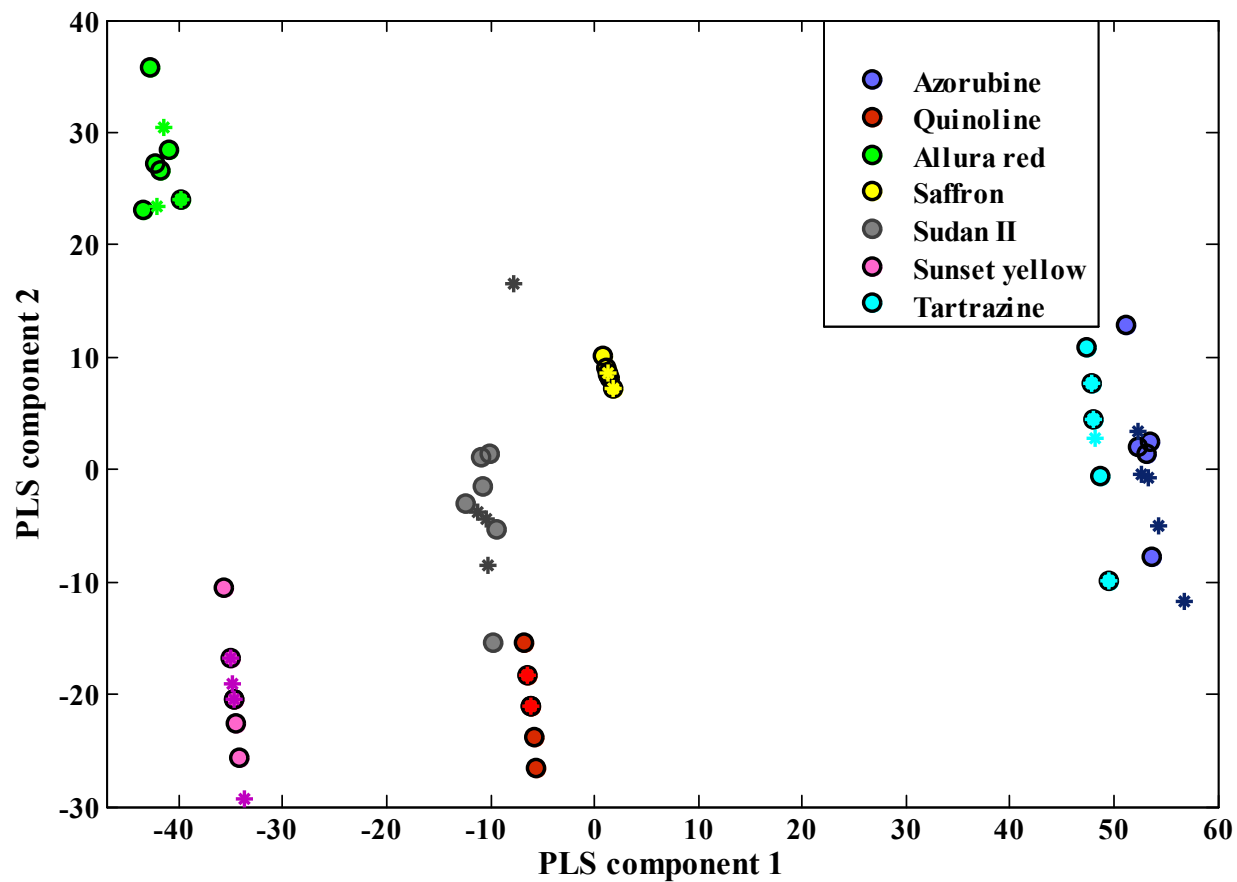


Figure (S4). Distribution pattern of the standard saffron and adulteration ones in the two-dimensional PLS-DA based factor space of their transmittance FT-IR spectra

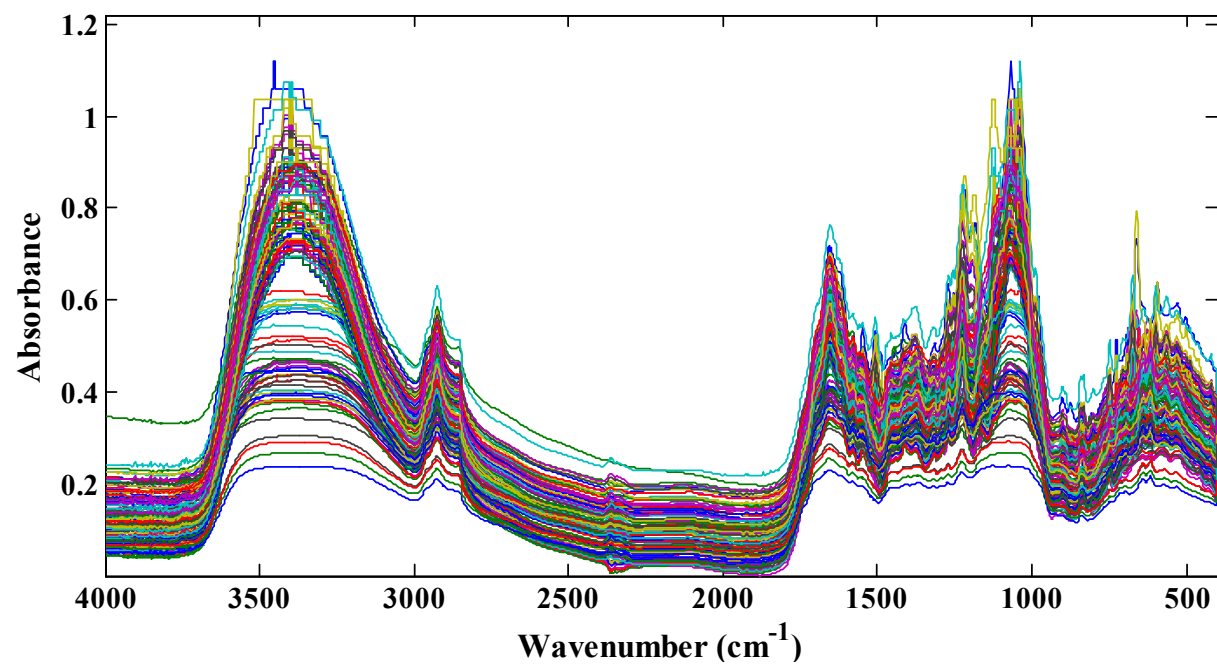


Figure (S5). Absorbance FT-IR spectra of food colorant adulteration in saffron samples