**Supplementary Materials**

**Optimizing TOF-SIMS and PCA Methods for Advanced Saffron Authenticity Screening: A Comprehensive Study**

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***Figure S1****. Positive and negative spectra of pure saffron powder analyzed with 0.1 pa Bi3+ current and a raster size of 500\*500 µm2.*



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***Figure S2****. Positive and negative spectra of pure safflower powder analyzed with 0.1 pa Bi3+ current and a raster size of 500\*500 µm2*



***Figure S3****. Positive and negative spectra of pure turmeric powder analyzed with 0.1 pa Bi3+ current and a raster size of 500\*500 µm2*

***Table S1****. proximate and photochemical composition of Saffron, Safflower and turmeric powders as reported in the literature and chemical structure of some compounds.*

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| --- | --- | --- |
| **Compound classification** | **Content**  **(in mg/g or in %)** | **Chemical structure**  **(with some proposed fragments)** |
| **Saffron (stigma)** | | |
| Carotenoids  (mostly crocin) | 6-16% | Crocetin with  R1 = R2 = Gentiobiosyl or Glucosyl sugar moiety  Gentiobiose, a rare disaccharide found in saffron and gentian, is a  reducing sugar and | StudySoupGentiobiose, a rare disaccharide found in saffron and gentian, is a  reducing sugar and | StudySoup |
| Terpenoid  (mostly picrocrocin: the glucoside precursor of safranal) | 1-13% |  |
| protein | 12-14% |  |
| pectin | 6-7% |  |
| Dextrin | 9-10% |  |
| Flavonoids (mostly reported anthocyanin and keampferol) | ~ 9.68 and 12.6 mg/g respectively | C:\Users\a.bejjani\AppData\Local\Microsoft\Windows\INetCache\Content.MSO\B9671777.tmpAnthocyanins: Structure, Properties, Sources and Uses |
| Minerals | K 8.2 🡪 12.2 mg/g  Mg 1.1 🡪 1.76 mg/g  P 3.2 🡪 4.4 mg/g |  |
| **Safflower (petals)** | | |
| Quinochalone  (Mostly Carthamin) | 0.83% |  |
| Flavonoid (kaempferol) | High content | C:\Users\a.bejjani\AppData\Local\Microsoft\Windows\INetCache\Content.MSO\B9671777.tmp |
| protein | 1.8% |  |
| Fatty acid  (Mostly linoleic acid (18:2), alpha linolenic acid (18:3) and palmitic acid (16:0)) | 4-8% | m/z=145🡪[169- C2H4]  m/z=409🡪 [437- C2H4]  m/z=465🡪[437+ C2H4]  m/z=493🡪 [437+ (C2H4)2]  m/z=521🡪[437+(C2H4)3] |
| Crude fibers | 11.6% |  |
| ash | 10.8% |  |
| Minerals | Ca 0.53 mg/g  Mg 0.287 mg/g  Fe 0.0073mg/g |  |
| stigmasterol | Reported as high content | Stigmasterol - Wikipedia |
| Beta-daucosterol | Reported as high content | Applied Sciences | Free Full-Text | Natural Sources, Pharmacological  Properties, and Health Benefits of Daucosterol: Versatility of Actions |
| **Turmeric (rhizome)** | | |
| Curcuminoids  (Mostly curcumin) | 2-15% | C:\Users\a.bejjani\AppData\Local\Microsoft\Windows\INetCache\Content.MSO\68A8A5E4.tmp |
| flavonoids | ~0.4 % |  |
| Essential oil | 3-7% |  |
| Carbohydrates | ~63% |  |
| water | ~13% |  |



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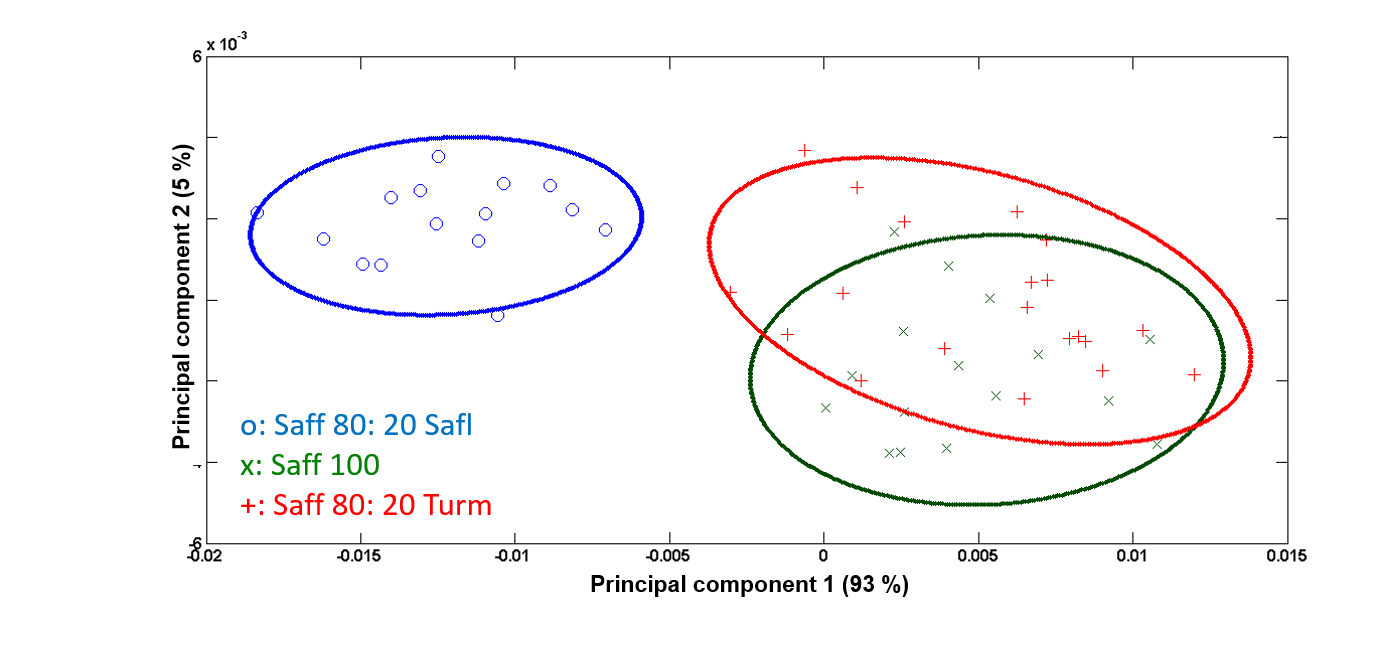
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**Figure S4**. *Positive spectra overlay of pure turmeric and saffron adulterated with 20% turmeric (inverted). The asterisk (\*) symbol denotes the signature peaks of curcumin molecule.*



**Figure S5**. *Positive spectra overlay of pure safflower and saffron adulterated with 20% safflower (inverted). The asterisk (\*) symbol denotes the signature peaks of turmeric*.



***Figure S6****. PC1 v/s PC2 scores plot of pure saffron (green), saffron adulterated with 20% of safflower (Saff80:20Safl, blue), and with turmeric (Saff80:20Turm, red). The ellipses around the points define the 95% confidence limit for each sample group*



***Figure S7****. PC1 v/s PC2 scores plot of pure saffron (Saf) and the three different groups of Saffron adulterated with 5%, 10% and 20% of Safflower (saffl)and the two groups of saffron adulterated with 5 and 20% of turmeric (Turm). The ellipses around the points define the 95% confidence limit for each sample group*