

Supplementary Material

Detection of Adulteration of Extra Virgin Olive Oil via Laser Induced Breakdown Spectroscopy and UV-Vis-NIR Absorption Spectroscopy: A Comparative Study

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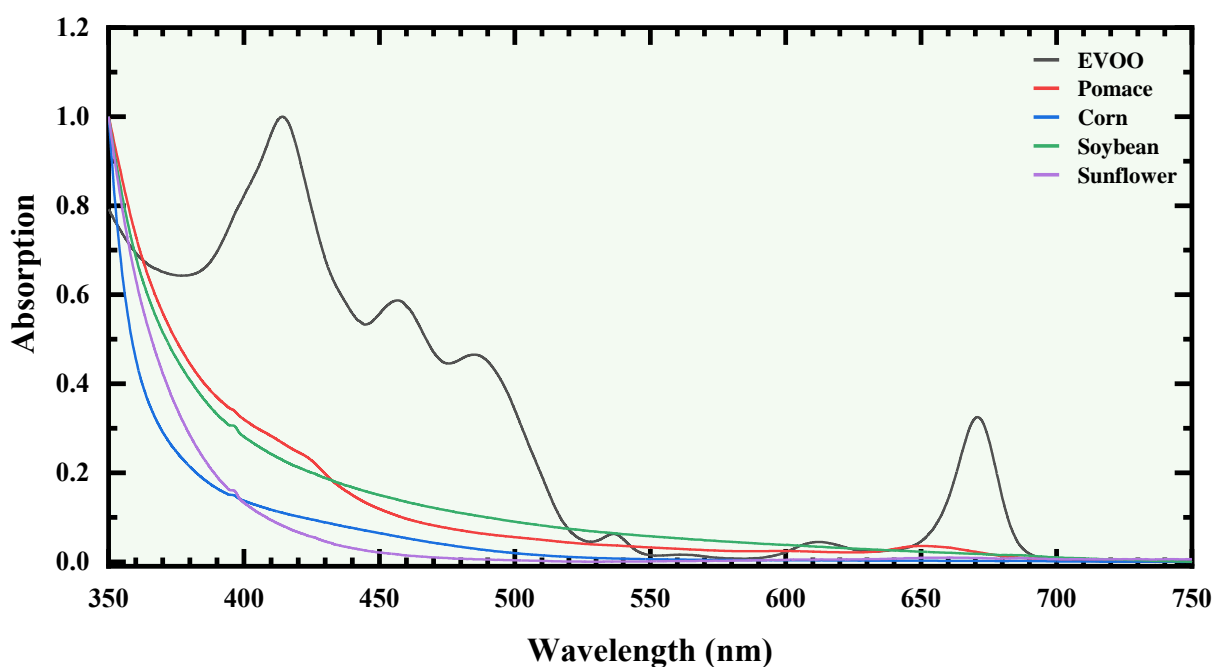


Figure S1. UV-Vis-NIR absorption spectra of an EVOO sample, pomace, corn, soybean, and sunflower oils

Table S1. Optimum number of PCs used for the analysis of the LIBS, UV-Vis-NIR absorption, and fused data by LDA, SVMs, and LR algorithms

		Optimum No. of PCs		
		LIBS	UV-Vis-NIR absorption	Fused data
All EVOOs and mixtures	LDA	70	20	60
	SVMs	30	10	50
	LR	30	10	80

EVOOs from Crete and mixtures	LDA	20	20	20
	SVMs	40	10	40
	LR	40	10	20
EVOOs from Lesvos and mixtures	LDA	40	10	20
	SVMs	20	20	30
	LR	20	10	60
EVOOs from Kalamata and mixtures	LDA	70	10	40
	SVMs	80	10	30
	LR	40	20	20
EVOOs from Achaia and mixtures	LDA	30	20	90
	SVMs	70	20	70
	LR	110	10	100

Table S2. Confusion matrices constructed for the SMVs algorithm, using the LIBS data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

SVMs algorithm						
Geographical origin	Actual class	Predicted class				
		EVOOs	Corn oil	Pomace oil	Soybean oil	Sunflower oil
Crete	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Lesvos	EVOOs	19	1	0	0	0
	Corn oil	0	18	2	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	1	19
Kalamata	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	1	19

Achaia	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	19	1	0
	Soybean oil	0	0	1	19	0
	Sunflower oil	0	0	0	0	20

Table S3. Confusion matrices constructed for the LR algorithm, using the LIBS data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

LR algorithm						
Geographical origin	Actual class	Predicted class				
		EVOOs	Corn oil	Pomace oil	Soybean oil	Sunflower oil
Crete	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	3	0	0	20
Lesvos	EVOOs	19	1	0	0	0
	Corn oil	0	19	0	1	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	1	19
Kalamata	EVOOs	20	0	0	0	0
	Corn oil	0	18	2	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	19	1
	Sunflower oil	0	0	0	3	17
Achaia	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	1	18	1
	Sunflower oil	0	0	0	0	20

Table S4. Confusion matrices constructed for the SVMs algorithm, using the UV-Vis-NIR absorption data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

SVMs algorithm						
Geographical origin	Actual class	Predicted class				
		EVOOs	Corn oil	Pomace oil	Soybean oil	Sunflower oil
Crete	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Lesvos	EVOOs	19	0	0	1	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Kalamata	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Achaia	EVOOs	10	0	10	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20

Table S5. Confusion matrices constructed for the LR algorithm, using the UV-Vis-NIR absorption data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

LR algorithm						
Geographical origin	Actual class	Predicted class				
		EVOOs	Corn oil	Pomace oil	Soybean oil	Sunflower oil
Crete	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0

	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Lesvos	EVOOs	19	0	0	1	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Kalamata	EVOOs	19	0	0	1	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Achaia	EVOOs	10	0	10	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20

Table S6. Confusion matrices constructed for the SVMs algorithm, using the fused data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

SVMs algorithm						
Geographical origin	Actual class	Predicted class				
		EVOOs	Corn oil	Pomace oil	Soybean oil	Sunflower oil
Crete	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	14	6
	Sunflower oil	0	0	0	0	20
Lesvos	EVOOs	20	0	0	0	0
	Corn oil	1	19	0	0	0
	Pomace oil	0	0	20	0	0

	Soybean oil	0	2	0	15	3
	Sunflower oil	0	0	0	0	20
Kalamata	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	17	3
	Sunflower oil	0	0	0	0	20
Achaia	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	16	0	0
	Soybean oil	0	0	0	19	1
	Sunflower oil	0	0	0	2	18

Table S7. Confusion matrices constructed for the LR algorithm, using the fused data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

LR algorithm						
Geographical origin	Actual class	Predicted class				
		EVOOs	Corn oil	Pomace oil	Soybean oil	Sunflower oil
Crete	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0
	Sunflower oil	0	0	0	0	20
Lesvos	EVOOs	20	0	0	0	0
	Corn oil	0	18	2	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	17	3
	Sunflower oil	0	0	0	1	19
Kalamata	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	20	0

	Sunflower oil	0	0	0	2	18
Achaia	EVOOs	20	0	0	0	0
	Corn oil	0	20	0	0	0
	Pomace oil	0	0	20	0	0
	Soybean oil	0	0	0	18	2
	Sunflower oil	0	0	0	1	19

Table S8. Precision and recall scores for the LDA, SVMs, and LR algorithms, using the LIBS, UV-Vis-NIR absorption, and fused data (where all EVOOs treated as one class while all EVOO-edible oil mixtures treated as another class)

			LIBS		UV-Vis-NIR absorption		Fusion	
			Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)
All EVOOs and mixtures	LDA	EVOOs	1	0.99	1	0.88	1	0.93
		Mixtures	1	1	0.97	1	0.98	1
	SVMs	EVOOs	1	0.99	1	0.99	1	0.99
		Mixtures	1	1	1	1	1	1
	LR	EVOOs	1	0.99	1	0.99	0.94	1
		Mixtures	1	1	1	1	1	0.98

Table S9. Precision and recall scores for the LDA, SVMs, and LR algorithms, using the LIBS data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

		LDA		SVMs		LR	
		Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)
LIBS	Crete	EVOOs	1	1	1	1	1
		Corn oil	1	1	1	1	1
		Pomace oil	0.9	0.9	1	1	1
		Soybean oil	1	1	1	1	1
		Sunflower oil	0.9	0.8	1	1	1
	Lesvos	EVOOs	1	1	1	0.95	0.95
		Corn oil	0.9	1	0.95	0.9	0.95
		Pomace oil	1	0.9	0.91	1	1
		Soybean oil	1	1	0.95	1	1

	Sunflower oil	1	0.9	1	0.95	1	0.95
	EVOOs	1	1	1	1	1	1
	Corn oil	1	0.9	1	1	1	0.9
Kalamata	Pomace oil	1	1	1	1	0.91	1
	Soybean oil	0.9	1	0.95	1	0.86	0.95
	Sunflower oil	1	0.9	1	0.95	0.94	0.85
	EVOOs	1	1	1	1	1	1
	Corn oil	1	1	1	1	1	1
Achaia	Pomace oil	1	1	0.95	0.95	0.95	1
	Soybean oil	1	0.9	0.95	0.95	1	0.9
	Sunflower oil	1	1	1	1	0.95	1

Table S10. Precision and recall scores for the LDA, SVMs, and LR algorithms, using the UV-Vis-NIR absorption data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

		LDA		SVMs		LR	
		Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)
UV-Vis-NIR absorption	EVOOs	1	0.9	1	1	1	1
	Corn oil	1	1	1	1	1	1
	Crete	Pomace oil	0.9	1	1	1	1
		Soybean oil	1	1	1	1	1
		Sunflower oil	1	1	1	1	1
	EVOOs	1	1	1	0.95	1	1
	Corn oil	1	1	1	1	1	1
	Lesvos	Pomace oil	1	1	1	1	1
		Soybean oil	1	1	0.95	1	1
		Sunflower oil	1	1	1	1	1
	EVOOs	1	1	1	1	1	0.95
	Corn oil	1	1	1	1	1	1
	Kalamata	Pomace oil	1	1	1	1	1
		Soybean oil	1	1	1	0.95	1
		Sunflower oil	1	1	1	1	1
	EVOOs	1	0.5	1	0.5	1	0.5
	Corn oil	1	1	1	1	1	1
	Achaia	Pomace oil	0.7	1	0.67	1	1
		Soybean oil	1	1	1	0.67	1
		Sunflower oil	1	1	1	1	1

Table S11. Precision and recall scores for the LDA, SVMs, and LR algorithms, using the fused data (where all the EVOOs from each region treated as one class while the EVOO-edible oil mixtures treated as four classes)

		LDA		SVMs		LR	
		Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)	Precision	Recall (Sensitivity)
Fusion	EVOOs	1	1	1	1	1	1
	Corn oil	1	1	1	1	1	1
	Crete Pomace oil	1	1	1	1	1	1
	Soybean oil	1	1	1	0.7	1	1
	Sunflower oil	1	1	0.77	1	1	1
	EVOOs	1	1	0.95	1	1	1
	Corn oil	1	1	0.90	0.95	1	0.9
	Lesvos Pomace oil	1	1	1	1	0.91	1
	Soybean oil	0.9	0.8	1	0.75	0.94	0.85
	Sunflower oil	0.8	0.9	0.87	1	0.86	0.95
	EVOOs	1	1	1	1	1	1
	Corn oil	1	1	1	1	1	1
	Kalamata Pomace oil	1	1	1	1	1	1
	Soybean oil	1	0.9	1	0.85	0.91	1
	Sunflower oil	1	1	0.87	1	1	0.9
	EVOOs	1	1	1	1	1	1
	Corn oil	1	1	0.83	1	1	1
	Achaia Pomace oil	1	1	1	0.8	1	1
	Soybean oil	0.8	0.8	0.90	0.95	0.95	0.9
	Sunflower oil	0.8	0.8	0.95	0.9	0.90	0.95