

Characterization and Classification of Spanish Honey by Non-targeted LC-HRMS (Orbitrap) Fingerprinting and Multivariate Chemometric Methods

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Table S1. Multiclass predictions by cross-validation for the set of honeydew-honey samples using 3 LVs. HO: Holm oak; MO: Mountain; and FO: Forest.

Sample class variety	Sensitivity (%)	Specificity (%)	Classification Error (%)
HO	100	100	0
MO	100	100	0
FO	100	100	0

Table S2. Number of analyzed honey samples considering botanical varieties and geographical origins.

Honey	Botanical variety	Number of samples	Geographical origin	Number of samples
Blossom-honeys	Orange/Lemon Blossom (BL)	12	Aragon	1
			Balearic Islands	2
			Cantabria	1
			Castile and Leon	2
			Catalonia	3
			Extremadura	1
			Spain ^a	2
	Eucalyptus (EU)	13	Andalusia	1
			Asturias	2
			Cantabria	1
			Castile and Leon	2
			Catalonia	1
			Extremadura	4
			Navarre	1
			Spain and others ^a	1
	Rosemary (RO)	26	Andalusia	1
			Aragon	4
			Asturias	1
			Balearic Islands	4
			Castile and Leon	1
			Cantabria	2
			Catalonia	6
			Extremadura	4
	Thyme (TH)	7	Navarre	1
			Spain ^a	2
			Castile and Leon	1
			Castile La Mancha	2
	Heather (HE)	18	Catalonia	1
			Extremadura	2
			Spain ^a	1
			Asturias	2
			Basque Country	1
			Cantabria	3
Honeydew-honeys	Mountain (MO)	6	Castile and Leon	5
			Catalonia	2
			Extremadura	5
			Spain ^a	1
	Forest (FO)	10	Castile and Leon	1
			Castile La Mancha	1
			Catalonia	2
			Balearic Islands	2
			Cantabria	2
	Holm Oak (HO)	10	Castile and Leon	1
			Catalonia	1
			Spain ^a	4
Other honeys	Multifloral (MF)	34	Aragon	2
			Castile and Leon	2
			Extremadura	6
			Asturias	1
			Balearic Islands	4
			Cantabria	1
			Castile and Leon	7
			Castile La Mancha	2
			Catalonia	8
			Extremadura	4
			Navarre	4
			Spain ^a	1
			Spain and others ^a	2

^a Spain: Honeys produced in Spain but geographical region not specified; Spain and others: Honeys that include mixtures of honey produced in Spain and other countries such as Uruguay, Cuba, Mexico, Romania or Ukraine

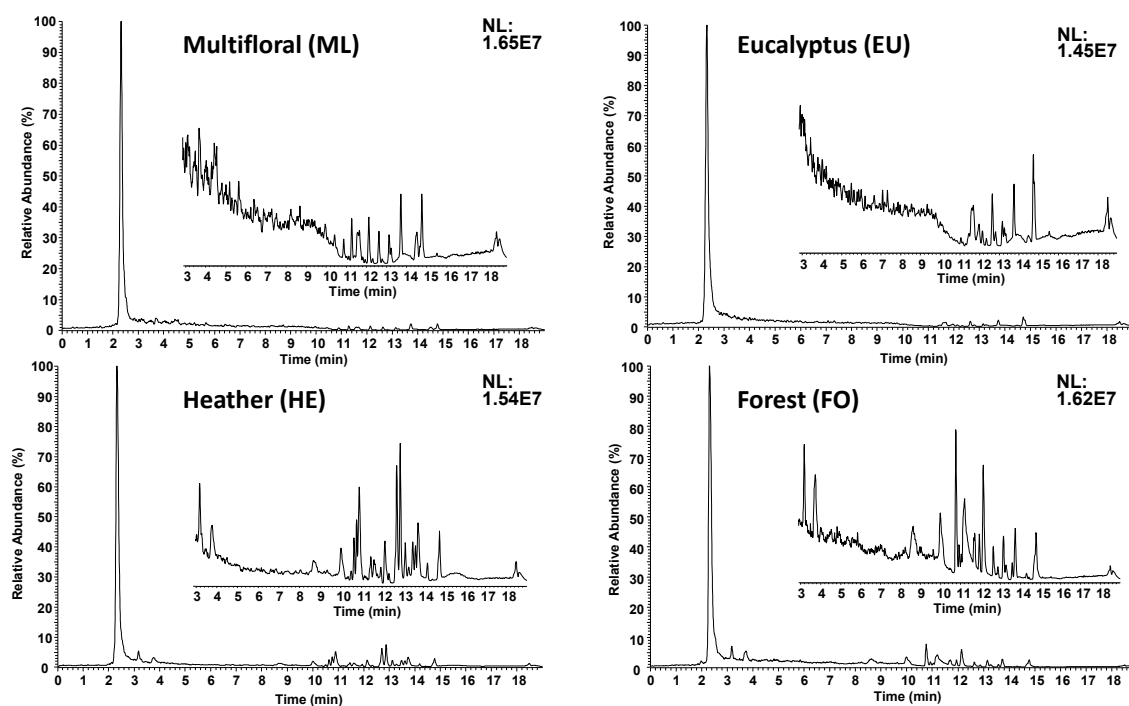


Figure S1. Non-targeted LC-HRMS (base peak chromatogram) fingerprints obtained for multifloral, eucalyptus, heather, and forest honeys.

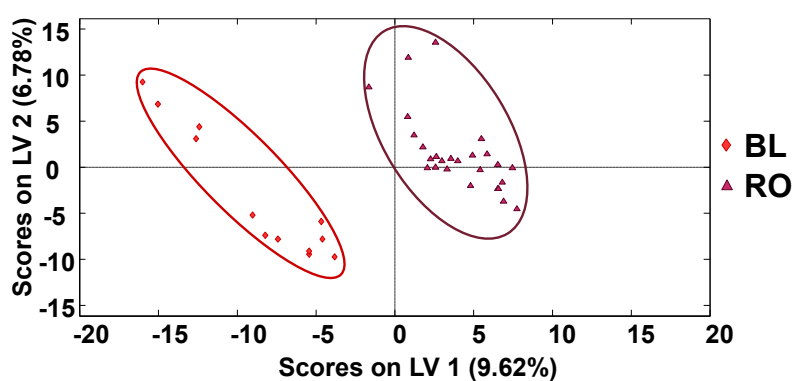


Figure S2. Supervised PLS-DA score plots of LV1 *vs.* LV2 when using non-targeted LC-HRMS fingerprints as honey chemical descriptors of orange/lemon blossom (BL) *vs.* rosemary (RO) blossom honeys (2 LVs were used to build the model).

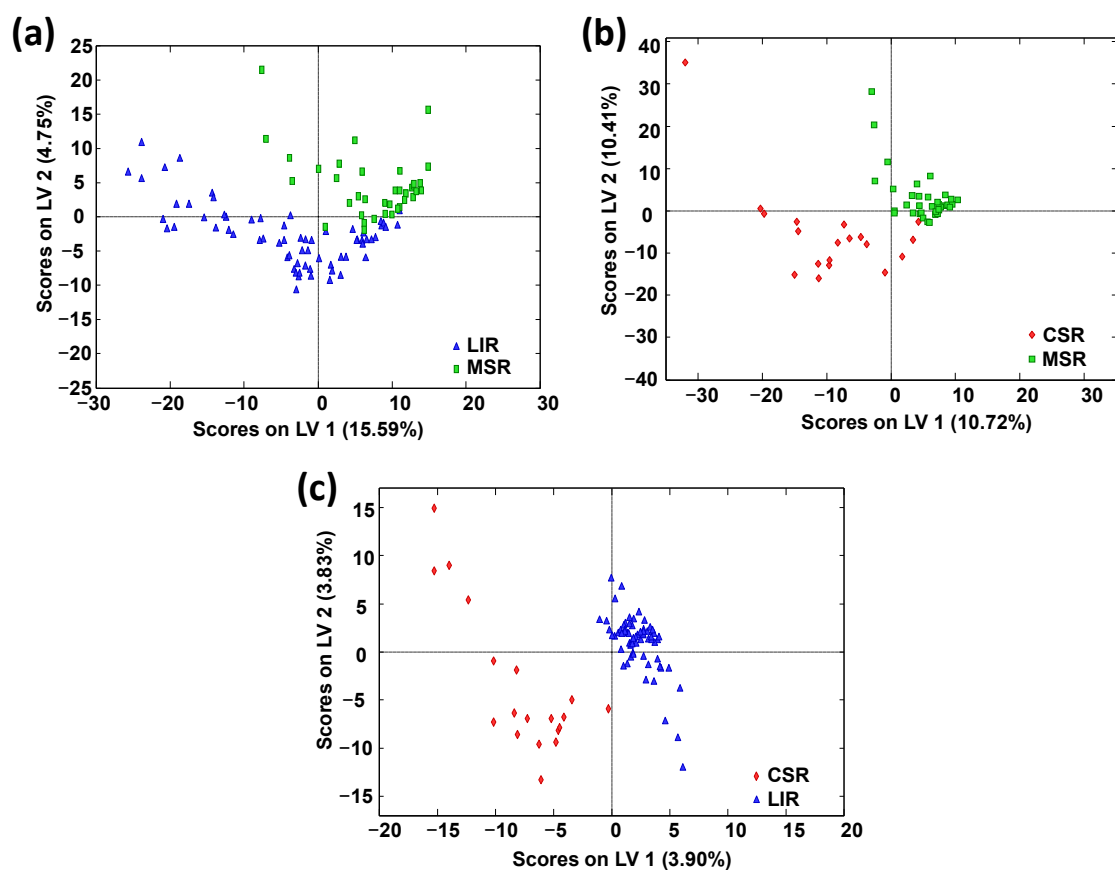


Figure S3. Paired PLS-DA score plots of LV1 vs. LV2 when using non-targeted LC-HRMS fingerprints as honey chemical descriptors of climatic geographical production region. (a) LIR *vs.* MSR (3 LVs were used to build the model), (b) CSR *vs.* MSR (2 LVs were used to build the model), and (c) CSR *vs.* LIR (2 LVs were used to build the model). CSR: Cantabrian Sea region; LIR: Landlock Inland region; MSR: Mediterranean Sea region.