

SUPPORTING INFORMATION

ION MOBILITY SPECTROMETRY VERSUS CLASSICAL PHYSICO- CHEMICAL ANALYSIS FOR ASSESSING THE SHELF LIFE OF EXTRA VIRGIN OLIVE OIL ACCORDING TO CONTAINER TYPE AND STORAGE CONDITIONS

Rocío Garrido-Delgado,¹ M. Mar Dobao-Prieto,¹ Lourdes Arce,¹ Joaquín Aguilar,² José
L. Cumplido,² Miguel Valcárcel^{1,*}

*¹Department of Analytical Chemistry, Faculty of Science, University of Cordoba,
Andalusian Institute of Fine Chemistry and Nanochemistry, International Agrifood
Campus of Excellence (ceiA3), Annex C3 Building, Campus of Rabanales, E-14071
Córdoba, Spain*

*²El Olivo Global, Pol. Industrial Tecnocórdoba, Glorieta de los Países Bálticos s/n
Building CFEUM, Nave 2, 14014 Córdoba, Spain*

**Corresponding author: Phone and Fax: +34 957 218616, E-mail: qa1meobj@uco.es*

Table S1. Signal Intensity, Expressed in Voltage, of Volatile Compounds (Mean and Standard Deviation) During Storage Under Household or Supermarket Conditions in Various Container Types, and ANOVA Results.

Volatile	Container		Household storage conditions					Market storage conditions				
		Month 1	Month 3	Month 5	Month 7	Month 9	Month 11	Month 3	Month 5	Month 7	Month 9	Month 11
2-Heptenal ^{1,2}	BB	0.253±0.016	0.275±0.003	0.321±0	0.368±0.002	0.404±0.014	0.370±0.007	0.293±0.005	0.296±0.012	0.382±0.002	0.393±0.02	0.368±0.022
	M	0.234±0.014	0.286±0.018	0.337±0.003	0.420±0.013	0.533±0.027	0.514±0.006	0.292±0.025	0.311±0.003	0.703±0.004	0.418±0.017	0.411±0.003
	DG	0.300±0.031	0.468±0.004	0.788±0.006	0.965±0.014	1.140±0.045	1.339±0.029	0.393±0.041	0.412±0.038	0.799±0.015	0.623±0.010	0.882±0.022
	CG	0.282±0.023	0.577±0.006	1.244±0.009	1.758±0.018	1.900±0.034	1.894±0.015	0.477±0.018	0.614±0.007	0.861±0.039	0.812±0.007	0.879±0.028
	PET	0.294±0.023	0.539±0.070	1.131±0.221	1.512±0.167	1.840±0.029	1.856±0.035	0.607±0.028	0.712±0.038	1.364±0.051	1.396±0.019	0.702±0.021
2-Penten-1-ol	BB	0.650±0.013	0.701±0.049	0.695±0	0.808±0.023	0.760±0.005	0.696±0.003	0.768±0.050	0.670±0.018	0.768±0.004	0.802±0.034	0.747±0.006
	M	0.609±0.044	0.679±0.010	0.693±0.006	0.741±0.024	0.790±0.015	0.682±0.004	0.704±0.035	0.690±0.032	0.721±0.009	0.811±0.013	0.745±0.016
	DG	0.648±0.046	0.671±0.017	0.694±0.013	0.721±0.002	0.715±0.008	0.669±0.010	0.681±0.025	0.667±0.021	0.783±0.004	0.745±0.020	0.765±0.017
	CG	0.677±0.060	0.663±0.025	0.709±0.016	0.772±0.006	0.808±0.013	0.731±0.013	0.714±0.025	0.661±0.021	0.817±0.011	0.766±0.012	0.784±0.021
	PET	0.731±0.059	0.661±0.014	0.684±0.003	0.613±0.137	0.687±0.029	0.633±0.006	0.691±0.012	0.690±0.015	0.794±0.014	0.740±0.017	0.754±0.004
Hexyl acetate	BB	0.231±0.009	0.248±0.005	0.239±0.003	0.259±0.006	0.242±0.008	0.192±0.006	0.247±0.006	0.233±0.004	0.266±0.004	0.253±0.011	0.186±0.006
	M	0.232±0.011	0.238±0.001	0.232±0.001	0.225±0.010	0.236±0.012	0.182±0.003	0.238±0.007	0.246±0.004	0.247±0.003	0.241±0.011	0.197±0.002
	DG	0.217±0.010	0.247±0.006	0.241±0.006	0.235±0.006	0.244±0.011	0.184±0.006	0.236±0.002	0.220±0.010	0.249±0.006	0.242±0.007	0.194±0.006
	CG	0.236±0.015	0.229±0.015	0.247±0.003	0.237±0.003	0.239±0.003	0.183±0.004	0.232±0.005	0.219±0.009	0.241±0.009	0.221±0.004	0.173±0.031
	PET	0.244±0	0.227±0.017	0.259±0.018	0.233±0.049	0.255±0.016	0.148±0.010	0.234±0.017	0.226±0.019	0.249±0.013	0.241±0.004	0.191±0.008
2-Hexenal	BB	3.985±0.009	4.049±0.004	4.063±0.001	4.087±0.012	4.152±0.017	3.979±0.031	4.006±0.036	3.997±0.023	4.158±0.006	4.072±0.014	4.094±0.015
	M	3.924±0.068	3.987±0.043	4.049±0.047	4.033±0.020	4.195±0.005	4.001±0.011	4.005±0.071	4.002±0.016	4.148±0.010	3.995±0.039	4.070±0.003
	DG	3.922±0.023	3.994±0.040	4.064±0.021	4.015±0.011	4.118±0.009	3.970±0.015	3.990±0.040	3.996±0.054	4.119±0.002	4.085±0.019	4.028±0.046
	CG	4.057±0.023	3.983±0.033	4.055±0.001	4.029±0.008	4.144±0.016	3.916±0.009	3.994±0.030	3.946±0.019	4.108±0.018	4.029±0.016	3.943±0.083
	PET	4.070±0.009	3.963±0.033	4.167±0.143	3.931±0.348	4.140±0.124	3.903±0.038	4.006±0.046	4.045±0.022	4.108±0.011	4.103±0.022	3.997±0.010
Hexanal ¹	BB	1.511±0.013	1.776±0.022	1.978±0.018	2.112±0.063	2.281±0.025	1.929±0.013	1.490±0.076	1.715±0.049	2.046±0.012	2.044±0.047	1.968±0.044
	M	1.266±0.164	1.606±0.137	1.905±0.099	1.941±0.049	2.262±0.017	1.831±0.021	1.555±0.105	1.649±0.040	2.001±0.006	1.968±0.069	1.953±0.014
	DG	1.325±0.035	1.724±0.134	2.028±0.011	2.025±0.042	2.114±0.046	1.798±0.019	1.634±0.155	1.894±0.211	2.191±0.004	2.408±0.021	2.083±0.040
	CG	1.595±0.034	1.565±0.115	1.913±0.001	2.230±0.058	2.373±0.059	1.907±0.012	1.696±0.129	1.691±0.057	2.307±0.057	2.193±0.040	2.074±0.082
	PET	1.651±0.019	1.602±0.138	1.883±0.097	1.682±0.312	1.988±0.187	1.520±0.013	1.701±0.153	1.779±0.038	2.105±0.019	2.193±0.071	1.995±0.003
Octanal ¹	BB	0.138±0.009	0.131±0.002	0.206±0.032	0.149±0.007	0.214±0.027	0.042±0.002	0.155±0.018	0.205±0.019	0.148±0.019	0.217±0.074	0.040±0.001
	M	0.196±0.070	0.174±0.017	0.235±0.040	0.139±0.002	0.205±0.016	0.043±0.002	0.191±0.031	0.197±0.017	0.151±0.008	0.174±0.064	0.043±0.002
	DG	0.149±0.020	0.170±0.023	0.261±0.050	0.152±0.009	0.229±0.021	0.045±0.002	0.163±0.014	0.178±0.028	0.212±0.022	0.325±0.025	0.044±0.004
	CG	0.138±0.006	0.172±0.009	0.336±0.009	0.233±0.012	0.316±0.014	0.046±0.002	0.158±0.008	0.178±0.014	0.260±0.037	0.270±0.011	0.047±0.003
	PET	0.190±0.041	0.165±0.014	0.314±0.039	0.165±0.012	0.240±0.042	0.044±0.002	0.169±0.016	0.184±0.015	0.217±0.004	0.260±0.032	0.042±0.001
1-Hexanol	BB	0.748±0.002	0.777±0.007	0.756±0.001	0.777±0.004	0.869±0.002	0.632±0.016	0.718±0.023	0.583±0.016	0.827±0.006	0.757±0.010	0.641±0.015
	M	0.731±0.045	0.746±0.015	0.741±0.041	0.746±0.021	0.855±0.001	0.627±0.005	0.732±0.042	0.585±0.009	0.821±0.007	0.726±0.015	0.635±0.006
	DG	0.711±0.011	0.738±0.020	0.752±0.010	0.748±0.016	0.796±0.010	0.605±0.005	0.718±0.030	0.576±0.032	0.800±0.005	0.842±0.009	0.627±0.006
	CG	0.778±0.022	0.706±0.026	0.733±0.004	0.740±0.019	0.816±0.008	0.606±0.008	0.726±0.019	0.567±0.009	0.803±0.018	0.783±0.003	0.607±0.021
	PET	0.795±0.014	0.713±0.007	0.750±0.036	0.767±0.104	0.805±0.080	0.592±0.021	0.733±0.027	0.593±0.007	0.810±0.003	0.838±0.007	0.632±0.006
1-Penten-3-one ^{1,2}	BB	2.706±0.019	2.690±0.009	2.484±0.012	2.596±0.027	2.508±0.011	2.460±0.007	2.682±0.100	2.557±0.009	2.655±0.012	2.478±0.013	2.564±0.010
	M	2.601±0.072	2.628±0.044	2.318±0.008	2.213±0.060	2.195±0.013	2.016±0.006	2.734±0.084	2.618±0.027	2.174±0.017	2.398±0.014	2.490±0.007
	DG	2.538±0.022	2.449±0.077	1.858±0.021	1.990±0.015	1.800±0.019	1.711±0.026	2.591±0.043	2.502±0.080	2.090±0.020	2.045±0.008	2.087±0.231
	CG	2.744±0.007	2.601±0.025	2.443±0.012	2.187±0.022	2.135±0.015	2.073±0.010	2.607±0.047	2.453±0.006	2.450±0.029	2.285±0.007	2.321±0.029
	PET	2.759±0.018	2.597±0.025	2.475±0.107	2.137±0.326	2.172±0.013	2.179±0.021	2.520±0.066	2.454±0.039	2.159±0.063	1.932±0.013	2.327±0.011
2-Hexen-1-ol	BB	0.410±0.010	0.424±0.005	0.410±0.004	0.454±0.002	0.410±0.015	0.336±0.007	0.446±0.048	0.362±0.007	0.439±0.006	0.450±0.037	0.345±0.017
	M	0.414±0.006	0.435±0.018	0.395±0.010	0.400±0.004	0.409±0.008	0.316±0.004	0.410±0.013	0.360±0.009	0.428±0.008	0.444±0.009	0.329±0.008
	DG	0.404±0.031	0.426±0.016	0.398±0.002	0.422±0.008	0.398±0.013	0.325±0.008	0.411±0.020	0.341±0.006	0.430±0.003	0.372±0.004	0.327±0.016
	CG	0.404±0.016	0.409±0.008	0.400±0.001	0.442±0.007	0.402±0.004	0.316±0.012	0.398±0.014	0.323±0.009	0.433±0.010	0.355±0.028	0.320±0.038
	PET	0.418±0.005	0.407±0.019	0.386±0.023	0.371±0.104	0.428±0.021	0.339±0.011	0.403±0.017	0.326±0.020	0.447±0.021	0.401±0.005	0.313±0.019
2-Pentenal ¹	BB	1.338±0.017	1.464±0.018	1.558±0.018	1.608±0.029	1.629±0.002	1.3980±0.015	1.317±0.040	1.361±0.057	1.654±0.007	1.420±0.022	1.482±0.018
	M	1.407±0.216	1.265±0.199	1.546±0.098	1.792±0.055	1.963±0.022	1.732±0.006	1.328±0.127	1.353±0.052	1.730±0.003	1.445±0.047	1.546±0.010
	DG	1.191±0.015	1.397±0.115	1.574±0.008	1.565±0.050	1.463±0.039	1.469±0.034	1.314±0.140	1.317±0.090	1.626±0.003	1.508±0.016	1.541±0.012
	CG	1.434±0.060	1.312±0.137	1.580±0.018	1.545±0.080	1.626±0.050	1.413±0.003	1.412±0.105	1.279±0.054	1.632±0.007	1.527±0.056	1.489±0.032
	PET	1.506±0.009	1.311±0.093	1.605±0.008	1.634±0.023	1.666±0.007	1.328±0.021	1.449±0.129	1.451±0.040	1.675±0.049	1.641±0.061	1.468±0.010

Superscript 1: volatile compounds exhibited significant differences in a one-way ANOVA in samples stored in previously opened containers (significance level < 0.5).

Superscript 2: there were significant differences in a one-way ANOVA in samples stored in closed containers (significance level < 0.5).

BB: bag-in-box, M: metal bottle, DG: dark glass bottle, CG: clear glass bottle, Pet: polyethylene terephthalate bottle.