

Chromatographic Fingerprinting by Template Matching for Data Collected by Comprehensive Two-Dimensional Gas Chromatography

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Materials

Name	Company	Catalog Number	Comments
¹ D SolGel-Wax column (100% polyethylene glycol; 30 m × 0.25 mm dc × 0.25 µm df). Carrier gas helium at a constant nominal flow of 1.3 mL/min.	Trajan SGE Analytical Science, Ringwood, Australia	PN 054796	Carrier gas helium at a constant nominal flow of 1.3 mL/min. Oven temperature programming set as follows: 40°C (2 min) to 240°C (10 min) at 3.5°C/min.
² D OV1701 column (86% polydimethylsiloxane, 7% phenyl, 7% cyanopropyl; 1 m × 0.1 mm dc × 0.10 µm df) from .	Mega, Legnano, Milan, Italy	PN MEGA-1701	
Automated system for sample preparation: SPR Autosampler for GC	SepSolve-Analytical, Llantrisant, UK		
Extra Virgin Olive oils: Sicily and Tuscany, Italy	Project VIOLIN (Ager - Fondazioni in rete per la ricerca agroalimentare)		Samples (n=10) were collected during the production year 2018 within the "Violin" project sampling campaign. Oils were submitted to HS-SPME to sample volatiles according to a reference protocol validated in a previous study of Stilo et al. ¹⁴
Gas chromatograph: Model 7890B GC	Agilent Technologies Wilmington DE, USA		
GC Image GC×GC edition V 2.9	GC Image LLC, Lincoln, Nebraska		https://www.gcimage.com/gcxgc/trial.html
Image processing software	GC Image LLC, Lincoln, Nebraska		https://www.gcimage.com/gcxgc/trial.html
Mass spectrometer: BenchTOF-Select	Markes International Llantrisant, UK		
Methyl-2-octynoate (CAS 111-12-6)	Merck-Millipore/Supelco	PN: 68982	
Modulator controller: Optimode v2.0	SRA Instruments, Cernusco sul Naviglio, Milan, Italy		
Modulator: KT 2004 loop type	Zoex Corporation Houston, TX, USA		

MS library and search software: NIST Library V 2017, Software V 2.3	National Institute of Standards and Technology (NIST), Gaithersburg MD		https://www.nist.gov/srd/nist-standard-reference-database-1a-v17
<i>n</i> -alkanes C8-C40 for retention indexing	Merck-Millipore/Supelco	PN: 40147-U	
<i>n</i> -hexane (CAS 110-54-3) gas chromatography MS SupraSolv	Merck-Millipore/Supelco	PN: 100795	
Solid Phase Microextraction fiber	Merck-Millipore/Supelco	PN 57914-U	
α - / β -thujone (CAS 546-80-5)	Merck-Millipore/Sigma Aldrich	PN: 04314	