

**Evaluation of extract backgrounds for
MRM-pesticides (QuEChERS) in fruits and
vegetables**

CONTENTS

1. Aim and scope	1
2. Short description.....	1
3. Procedure.....	1
3.1. Sample extraction	1
3.2. Instrumentation and analytical conditions for the LC-TOF-MS system.....	1
3.2.1. Agilent 1200 HPLC	1
3.2.2. Agilent 6530 LC-QTOF-MS.....	2
4. Number and distribution of co-extracted matrix components	2

1. Aim and scope

This report describes the evaluation of the background of six relevant Fruit and Vegetable commodities with different degrees of difficulty using LC-TOF-MS.

2. Short description

White grape, aubergine, tomato, red onion, leek and orange were extracted by citrate QuEChERS and analysed by LC-TOF-MS. Matrix compounds were retrieved and counted using the Molecular Feature Extractor (MFE) algorithm in the MassHunter Workstation Software. The MFE creates a compound list of all the peaks in the data file that represent real molecules. At the end of the data process, a list with the mass, retention time, and intensity of all matrix components was obtained. The resulting data was evaluated to get information of the complexity of the matrices thorough the number and distribution of the matrix components.

3. Procedure

3.1. Sample extraction

The buffered citrate QuEChERS method was applied to the six selected matrices.

3.2. Instrumentation and analytical conditions for the LC-TOF-MS

3.2.1. Agilent 1200 HPLC

- Column: Agilent XDB, C18, 4.6 mm x 50 mm x1.8 µm
- Mobile phase A: acetonitrile 0.1% Formic Acid 5% ultrapure water
- Mobile phase B: 0.1% Formic acid in ultrapure water
- Flow rate: 0.6 mL/min
- Injection volume: 10 µL

Mobile phase gradient

Time [min]	Mobile phase A	Mobile phase B
0	10%	90%
1	10%	90%
11	100%	0%
17	100%	0%

Re-equilibration with initial mobile phase: 7 minutes.

3.2.2. Agilent 6530 LC-QTOF-MS

- 4GHz High Resolution Mode
- ESI source gas temperature: 350°C
- Gas flow: 10 L/min
- Nebuliser gas and collision gas: nitrogen
- Nebuliser gas pressure: 40 psi
- Sheath gas flow: 12 L/min
- Sheath gas temperature: 400 °C
- Ionisation mode: positive
- Capillary voltage: 4000 V
- Skimmer voltage 65 V
- OctapoleRFPeak 750V
- Fragmentor 90 V

4. Number and distribution of co-extracted matrix components







