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LCMS QC Reference Material

CONTENTS

I. INTRODUCTION

The Quality Control Reference Materials (QCRM) portfolio is a unique collection of standards and mixtures. These products allow the user to evaluate and benchmark their chromatography system before analysis of critical material. The products in the portfolio are all specially formulated based on the expertise of Waters scientist.

The LCMS QCRM is a 9 component mix used to provide a comprehensive reference standard for use with LC/MS or MS instrumentation with a wide variety of conditions and methods.

- The compounds in this mix give a mixture of responses in ESi (+-) and APCi+
- Covers a wide range of m/z
- Optimized concentration to provide a more equal response by component in ESI+ mode
- Provides a separation in a range of chromatographic conditions used to benchmark instrument performance

Table 1. Individual Components in the LCMS QCRM Mix

Component	Empirical Formula	Exact Mass (as [M+H]+)	Exact Mass (as [M+H]–)	Concentration for analysis (µg/mL)
Acetaminophen	$C_8H_9NO_2$	152.0712	150.0555	10
Caffeine	$C_8H_{10}N_4O_2$	195.0882		1.5
Sulfaguanidine	$C_7H_{10}N_4O_2S$	215.0603	213.0446	5
Sulfadimethoxine	$C_{12}H_{14}N_4O_4S$	311.0814	309.0658	1
Val-Tyr-Val	$C_{19}H_{29}N_3O_5$	380.2185	378.2029	2.5
Verapamil	$C_{27}H_{38}N_2O_4$	455.2910		0.2
Terfenadine	$C_{32}H_{41}NO_2$	472.3216		0.2
Leucine-Enkephalin	$C_{28}H_{37}N_5O_7$	556.2771	554.2615	2.5
Reserpine	$C_{33}H_{40}N_2O_9$	609.2812		0.6

II. STORAGE AND STABILITY

The standard mix comes in a Waters Crimp Top vial for direct injection and contains 500 µL total in 1:10 in ACN:LC/MS Grade Water.

The standard mix is shipped at ambient temperatures. It is highly recommended that upon receipt, the standard should be refrigerated at 4 °C for short term and for long term stored frozen.

III. EXAMPLES OF USING THE LCMS QCRM

In this section, two example methods are discussed to allow the user to get an idea and understanding of how this standard can be used under different conditions. The user is not aiming for an exact replicate of these LC/MS chromatograms, however this is provided as guidance. The advantage of this standard is that it can be used with any column under different LC conditions. Therefore, based on the information shown below, the user can customize this standard to their specific method.

Shown in Figure 2 is a representative MS Spectrum under the following conditions listed in Table 2.:

Table 2: Gradient Table for Figure 1

Time/min	Flow rate/ mL min	%A	%B	Curve
0.0	0.5	100	0	–
3.5	0.5	0	100	6
4.5	0.5	100	0	11
Total analysis time = 5 min				

Column: ACQUITY® HSS T3, 2.1 x 100 mm, 1.8 µm
Mobile phase A: Water + 0.1 % formic acid
Mobile phase B: Acetonitrile
Injection volume: 1 µL

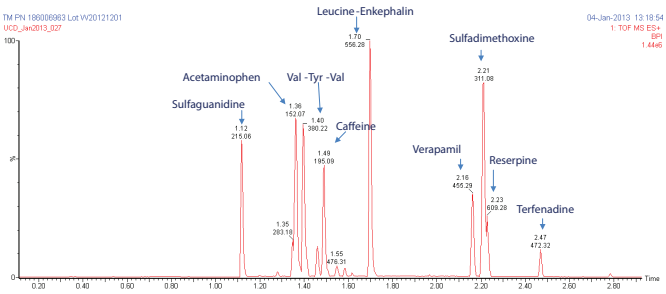

Figure 1: TOF MS ES+ Spectrum of the LCMS QCRM Standard using ACN Mobile Phase with a SYNAPT® G2-S MS operated in positive ion mode in high resolution mode

Table 3: Gradient Table for Figure 2

Time/min	Flow rate/ mL min	%A	%B	Curve
0.0	0.5	100	0	–
3.5	0.5	0	100	6
4.5	0.5	100	0	11
Total analysis time = 5 min				

Column: ACQUITY HSS T3, 2.1 x 100 mm, 1.8 µm
Mobile phase A: Water + 0.1 % Formic acid
Mobile phase B: Methanol + 0.1 % Formic acid
Injection volume: 1 µL

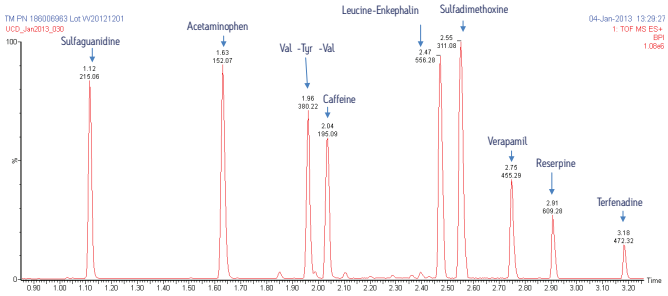

Figure 2: TOF MS ES+ Spectrum of the LCMS QCRM Standard using Methanol Mobile Phase with a SYNAPT G2-S MS operated in positive ion mode in high resolution mode

IV. ORDERING INFORMATION

Description	Part Number
LCMS QC Reference Standard	186006963
Neutrals QCRM	186006360
Reversed-Phase QCRM	186006363
Preparative Chromatography Mix Standard	186006703
HILIC QCRM	186007226
QDa QCRM	186007345
Quad LCMS QCRM	186007362
UPC^2 QCRM	186007950
AutoPurification System Standard	716000765

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Waters Corporation
34 Maple Street
Milford, MA 01757 U.S.A.
T: 1 508 478 2000
F: 1 508 872 1990
www.waters.com