

## Waters® Alliance® LC/MS System



Experiment Conditions  
Calibration Curves  
Results

### **Key Word:**

QuanLynx  
ZMD  
Quantitation  
Automation

1. Micromass Bruchure No. BR23.: QuanLynx...the software solution for automated LC-MS-MS method development and multi-compound quantification

## QuanLynx™ on Waters ZMD LC/MS System for Automated Methods Development

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QuanLynx is an integral function of the MassLynx™ software (version 3.3 or higher). It offers automated MS method development for quantitation using SIR or MRM. The automated process includes instrument optimization, data acquisition and quantification. QuanLynx can be implemented on tandem quadrupole instruments (Micromass® Quattro II™, Quattro LC™ and Quattro Ultima™) as well as single quadrupole instruments (Waters ZMD).

The application of QuanLynx on tandem quadrupole instruments has been shown elsewhere<sup>1</sup>. The purpose of this note is to demonstrate how QuanLynx can be utilized on a single quadrupole instrument such as the Waters ZMD. A mixture of Acetaminophen/Caffeine was used as the sample analyte. Manual quantitation of the mixture is also performed. The quantitation results by QuanLynx and by Manual quantitation are compared.

# Experiment Conditions

## HPLC:

System: Waters Alliance<sup>®</sup> 2690 with 996 PDA  
Column: Waters Symmetry<sup>®</sup> C<sub>18</sub>, 3.5 µm, 2.1 x 50 mm  
Mobile Phase: MeOH/H<sub>2</sub>O 30/70 Isocratic  
Injection Volume: 10 µL  
Flow Rate: 0.2 mL/min.

## MS:

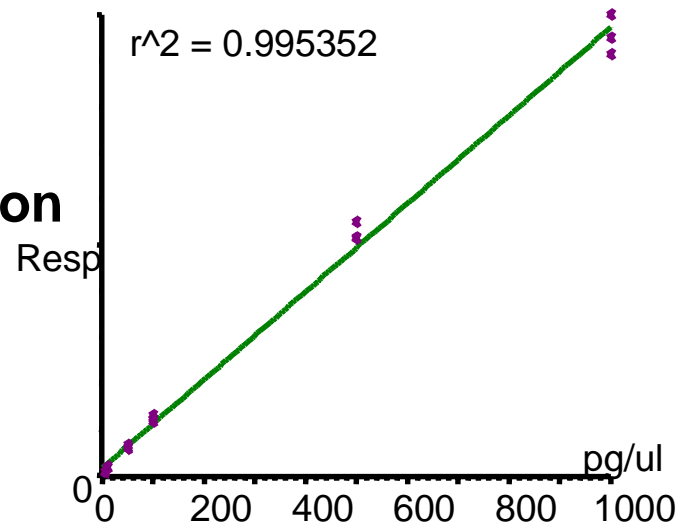
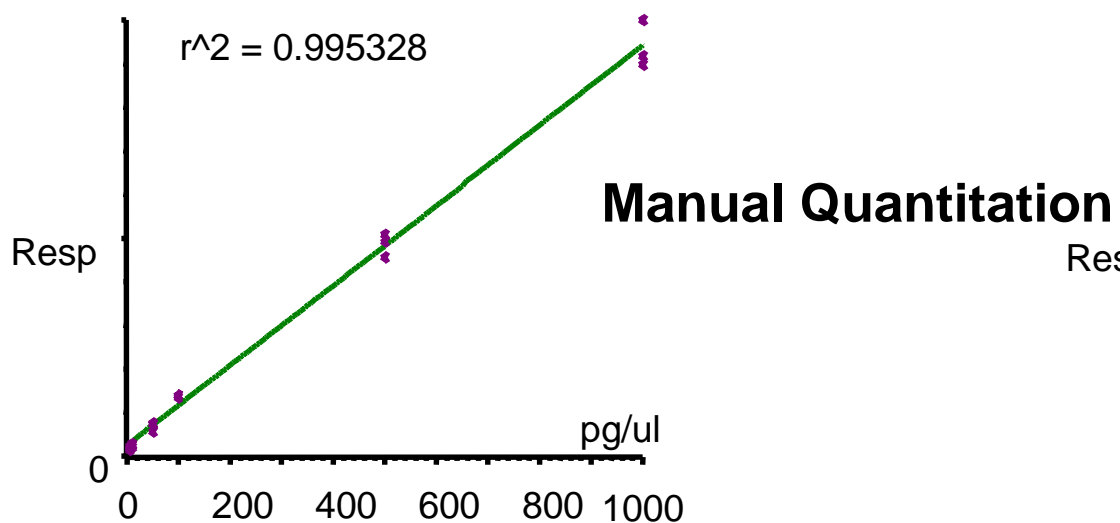
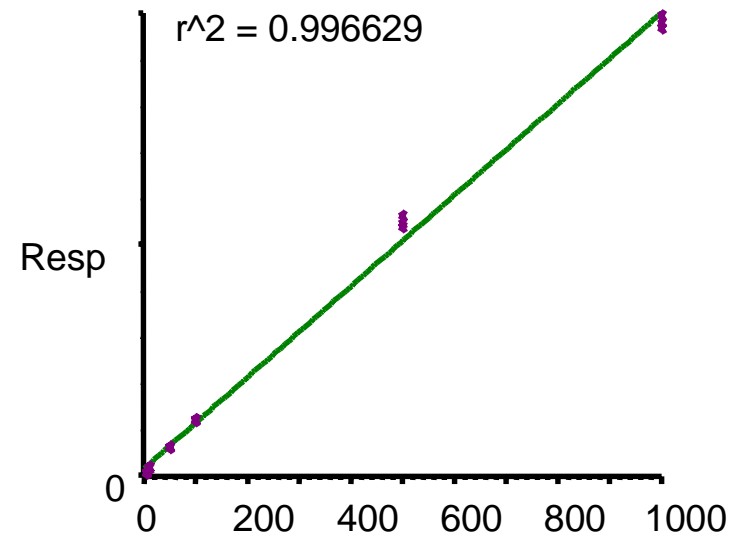
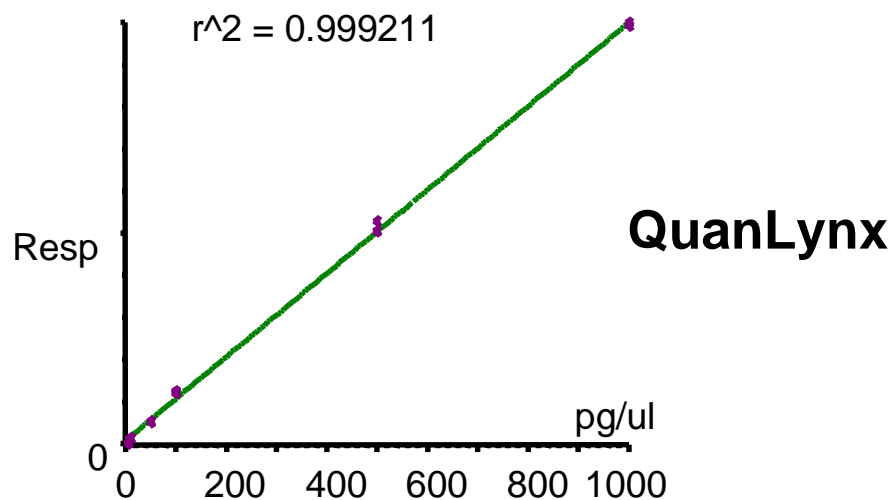
System: Waters ZMD  
Ionization Mode: ESI+

**Results on the next two pages show that in addition to saving in time, QuanLynx also offers better precision and accuracy, compared to manual quantitation.**

# Comparison of Calibration Curves

## Acetaminophen

## Caffeine



# Comparison of Results

		Acetaminophen		Caffeine	
		QuanLynx	Manual	QuanLynx	Manual
<b>Mean</b>	<b>L1</b>	219.1	220.7	227.7	229.7
<b>(pg/μL)</b>	<b>L2</b>	73.4	82.1	78.2	80.6
<b>SD</b>	<b>L1</b>	1.15	9.70	1.20	10.3
	<b>L2</b>	3.65	5.44	2.68	4.71
<b>%CV</b>	<b>L1</b>	0.53	4.40	0.53	4.48
	<b>L2</b>	4.97	6.63	3.42	5.85
<b>% Error</b>	<b>L1</b>	9.55	10.4	13.8	14.8
	<b>L2</b>	-2.13	9.47	4.26	7.46
<b>LOD (pg/μL)</b>		10.7	9.21	6.84	14.4
<b>LOQ (pg/μL)</b>		35.6	30.7	22.8	48.0
<b>r<sup>2</sup></b>		0.999	0.995	0.997	0.995