Opiates, Opioids and Benzodiazepines, Amphetamines & Illicit Drug Forensic Analysis by LC/MS
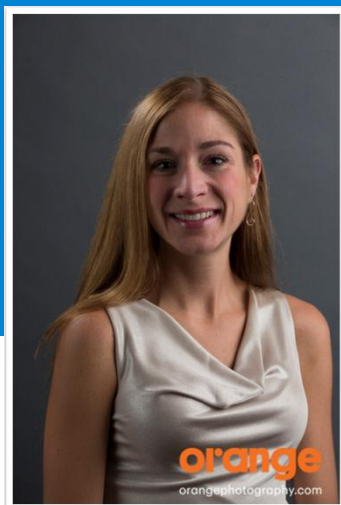
Julie Cichelli, PhD

Agilent Technologies

Application Engineer

April 29, 2014
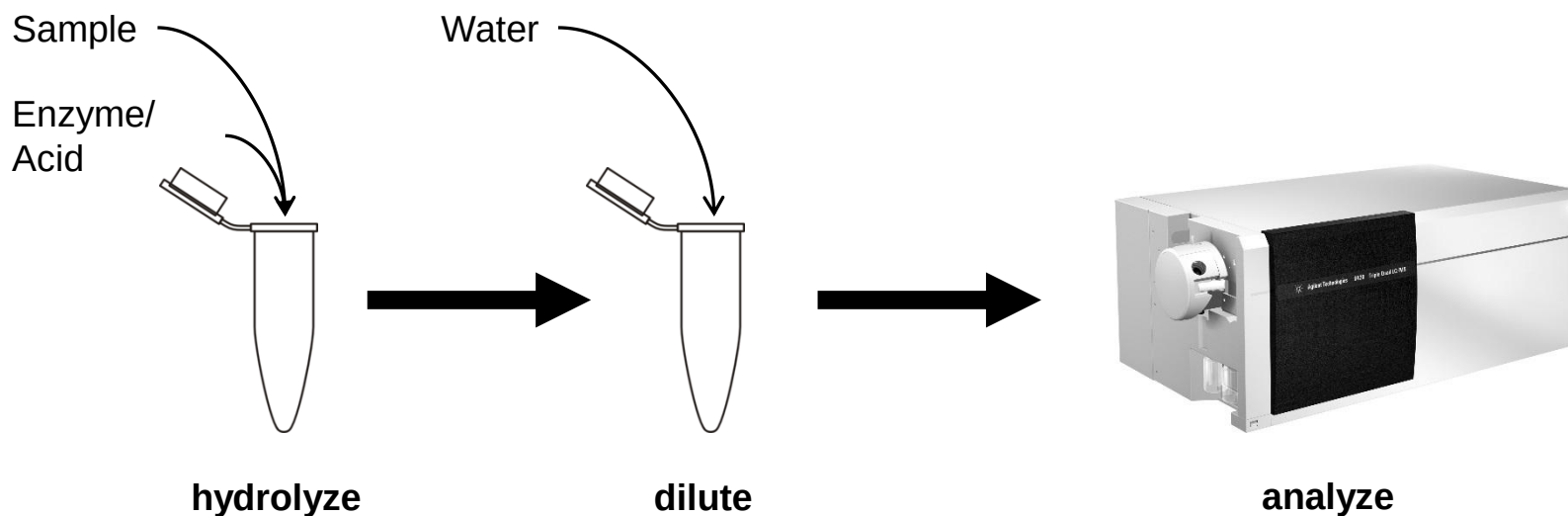
Agenda

- A method for the rapid analysis of over 65 analytes in a single LC/MS analysis run

- Simplified method development through the use of Dynamic MRM (dMRM) and databases

- Qualitative and Quantitative data analysis

- Customized Reporting

Agilent Technologies

For Forensic Use.
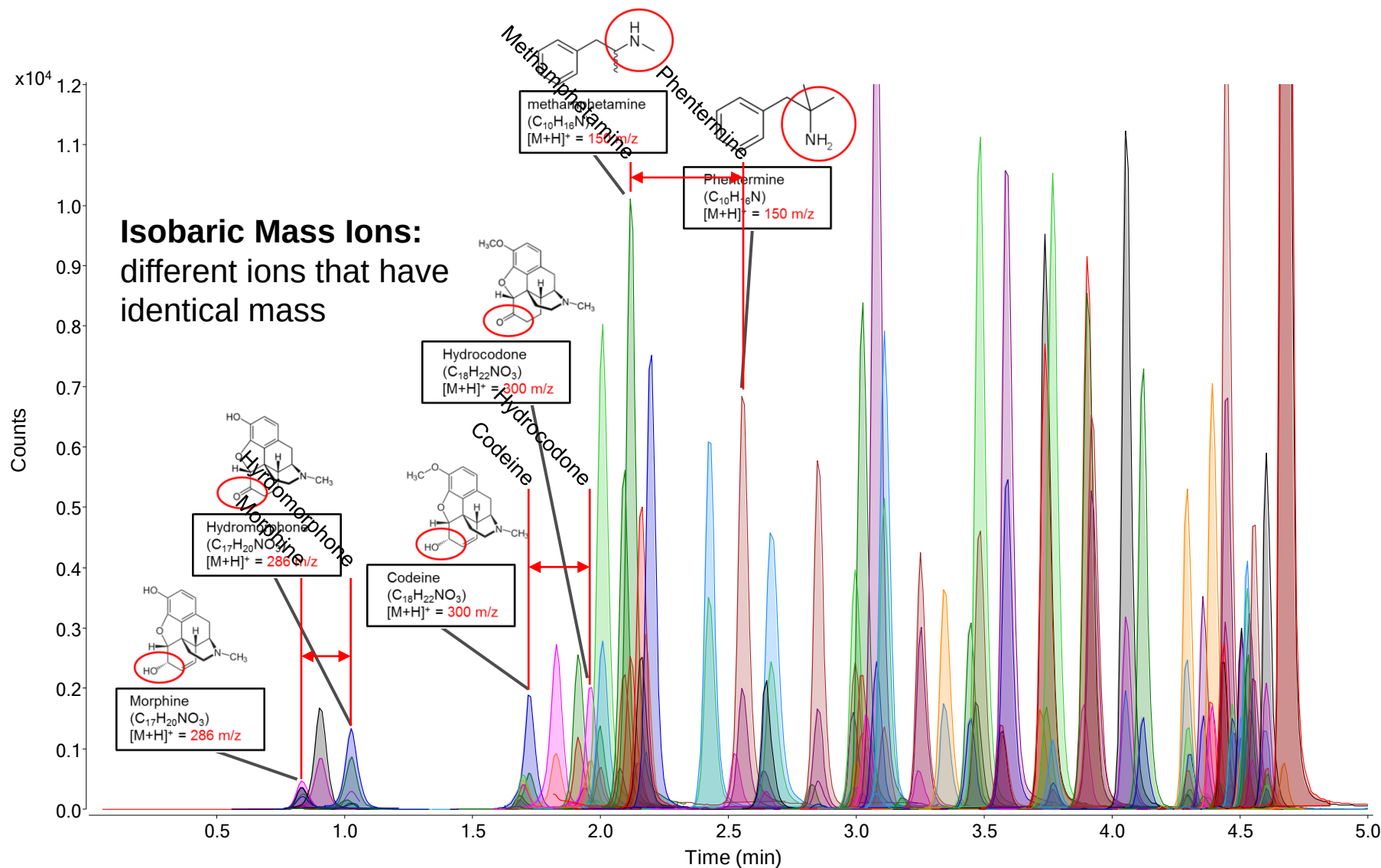
# Targeted Analysis of Over 65 Analytes for Toxicology

- An extensive screen and quantification in 5 to 6 minutes
- Internal standard corrected quantification
- Multi-point calibration curve covering a wide dynamic range
- Secondary qualifier ion for each analyte
- Simple sample preparation:

Sample

Water

Enzyme/
Acid

hydrolyze   **dilute**   **analyze**

Chromatographic Separation of Over 65 Analytes

Isobaric Mass Ions: different ions that have identical mass

methamphetamine
($C_{10}H_{16}N$)
$[M+H]^+$ = 150 m/z

Phentermine
($C_{10}H_{16}N$)
$[M+H]^+$ = 150 m/z

Hydrocodone
($C_{18}H_{22}NO_3$)
$[M+H]^+$ = 300 m/z

Hydromorphone
($C_{17}H_{20}NO_3$)
$[M+H]^+$ = 286 m/z

Codeine
($C_{18}H_{22}NO_3$)
$[M+H]^+$ = 300 m/z

Morphine
($C_{17}H_{20}NO_3$)
$[M+H]^+$ = 286 m/z

Counts

Time (min)

Agilent Technologies

For Forensic Use.
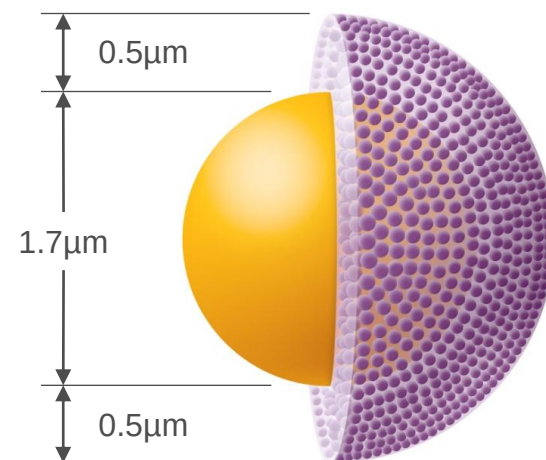
Poroshell 120 Columns for HPLC and UHPLC

Poroshell 120 is a high efficiency, high resolution column choice for enhancing productivity in LC and LC/MS

Poroshell 120 Columns have:

*   80-90% efficiency of sub-2μm columns

*   ~40-50% lower pressure

*   2x efficiency of 3.5μm (totally porous)

*   A 2μm frit to reduce clogging

*   A 600 bar pressure limit for HPLC or UHPLC

*   The superficially porous particle is 2.7um with a solid core (1.7um) and porous outer layer with a 0.5um diffusion path

0.5μm

1.7μm

0.5μm

Poroshell 120 Performance After 3000 Injections
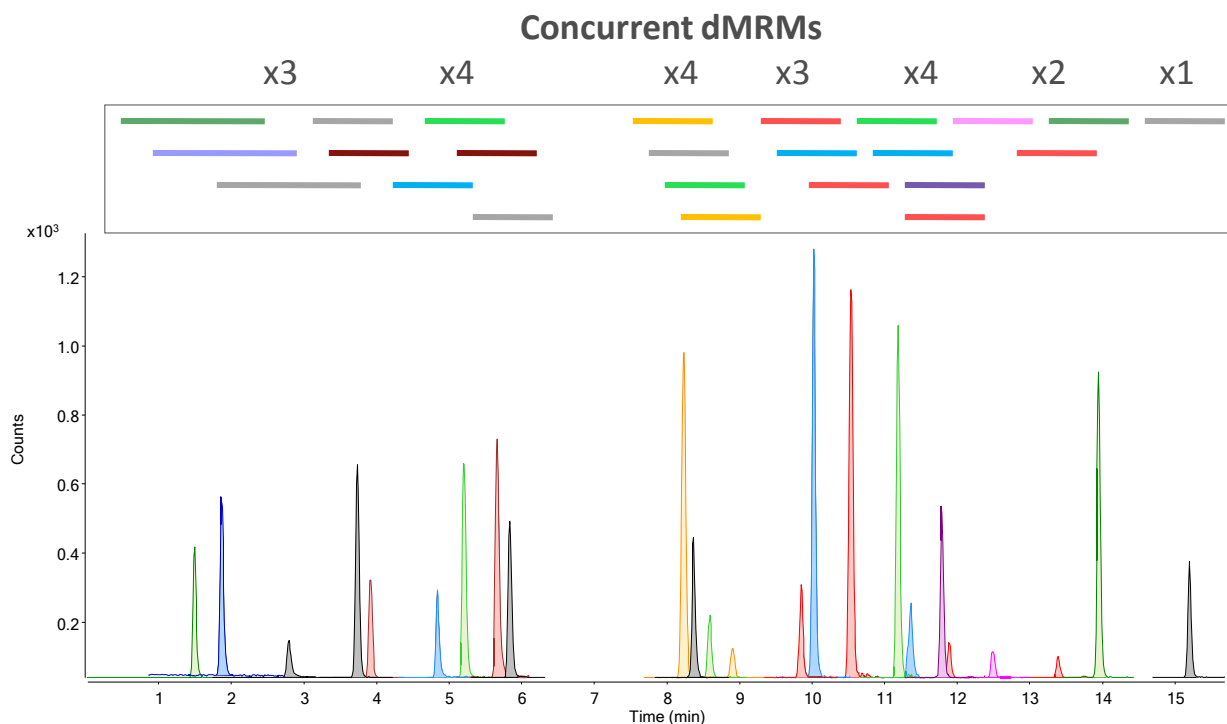
- Dilute and shoot sample preparation
- Analytes covering a wide range of retention times show excellent reproducibility

Analyte	%RSD (RT)	Analyte	%RSD (RT)	Analyte	%RSD (RT)
Morphine	0.7	Meperidine	0.4	Triazolam	0
Codeine	0.4	zolpidem	0.3	Naltrexone	0.1
hydrocodone	0.4	Fentanyl	0.1	chlordiazepoxide	0.1
MDMA	0.3	EDDP	0.1	Desmethyl diazepam	0.1
norFentanyl	0.2	Nitrazepam	0.1	Buprenorphine	0.3
Heroin	0.2	Propoxephine	0.1	Cocaethylene	0.2
Methyl Phenidate	0.2	Buprenorphine	0.3	11-nor-9-carboxy-delta9-thc	0

The Need for Dynamic MRM (dMRM)

- Nearly 200 MRM transitions for analytes, qualifier ions, and internal standards
- Monitoring all MRM transitions over the entire run results in poor quantification due to short dwell times and long cycle times
- dMRM only monitors each transition during the appropriate retention time window

Easy LC/MS Method Creation and Customization
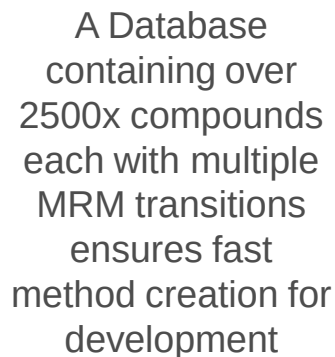
Agilent Analyzers and Application Kits

Triple Quadrupole LC/MS
Forensic Toxicology Application Kit

Quickly and efficiently implement target screening methods

A Database containing over 2500x compounds each with multiple MRM transitions ensures fast method creation for development

Quickly establish screening methods for complex matrices using these leading-edge technologies

A Dynamic MRM database with more than 200 compounds, plus **Agilent MassHunter Data Acquisition and Analysis software,** let you quickly generate acquisition and analysis methods, which can be modified to meet your future needs.

The Agilent 1200 Series SL Rapid Resolution LC, interfaced with Agilent's 6400 Series Triple Quadrupole LC/MS System delivers fast, high-resolution LC/MS/MS analysis.

Agilent's Jet Stream Electrospray lowers detection levels of analytes in complex matrices.

Dynamic MRM maximizes the Quadrupole's detection capability – without sacrificing sensitivity – when a large number of compounds are being analyzed at femtomole concentrations.
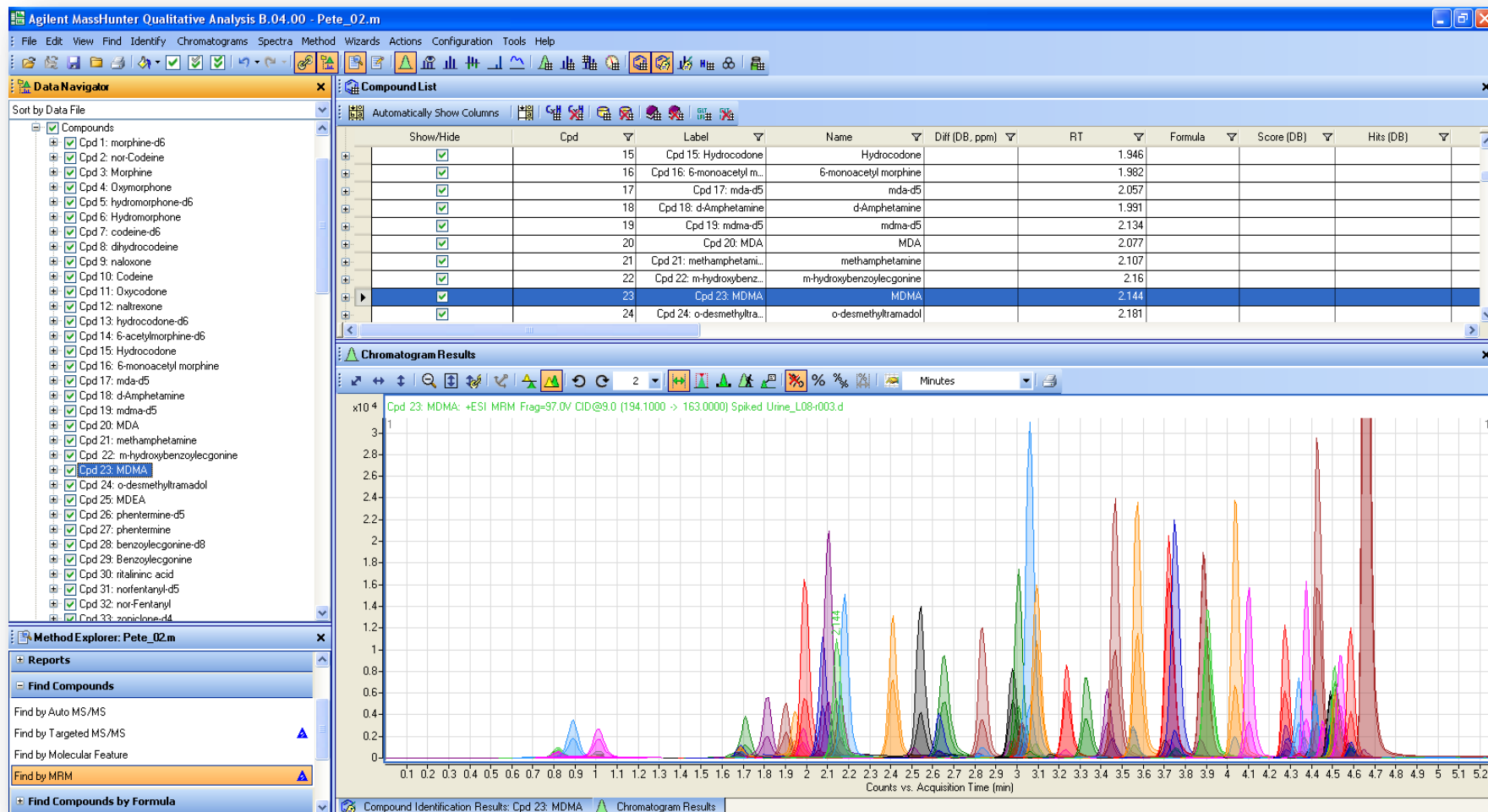
Qualitative Screening
Find By MRM
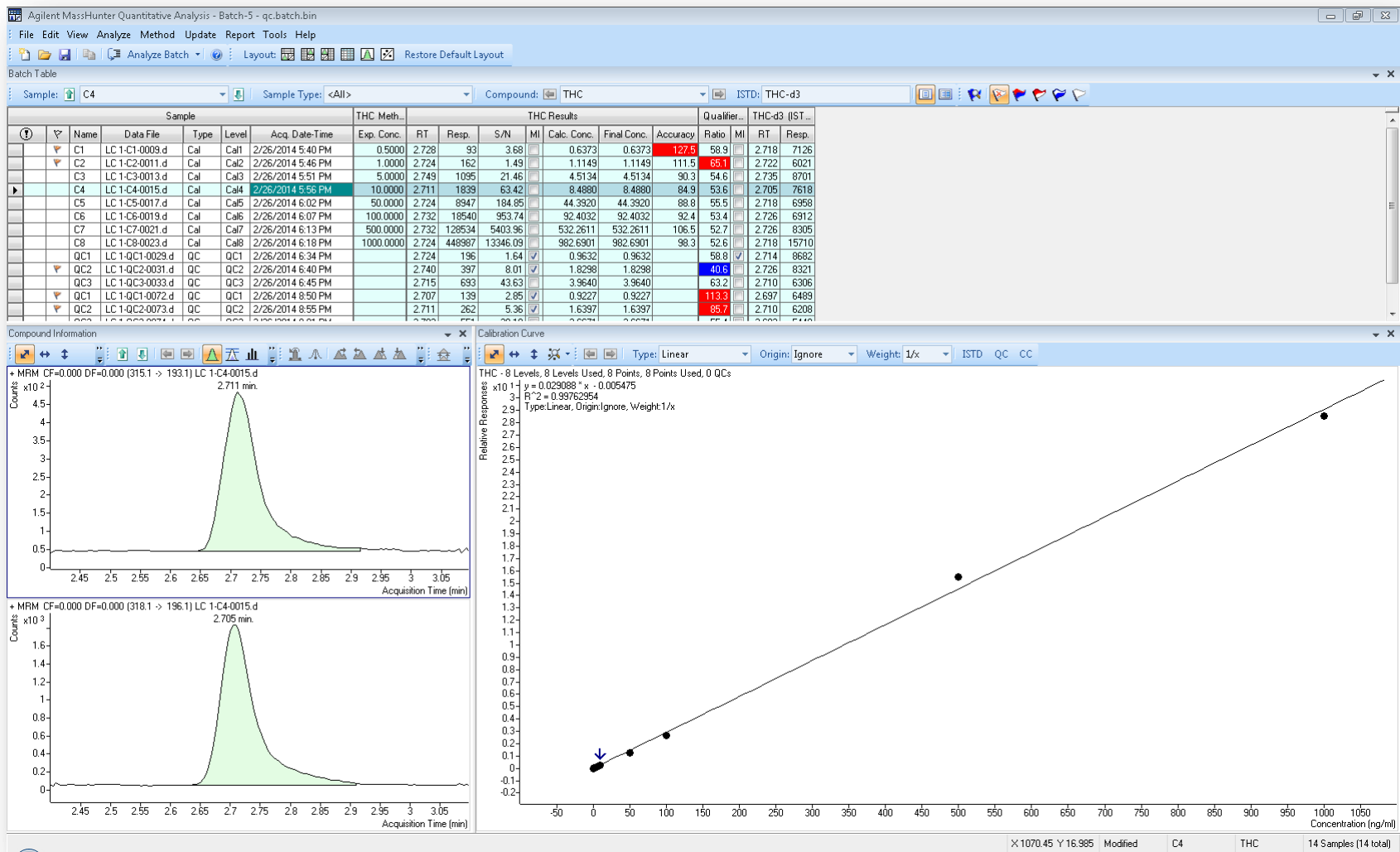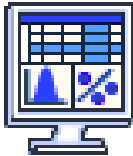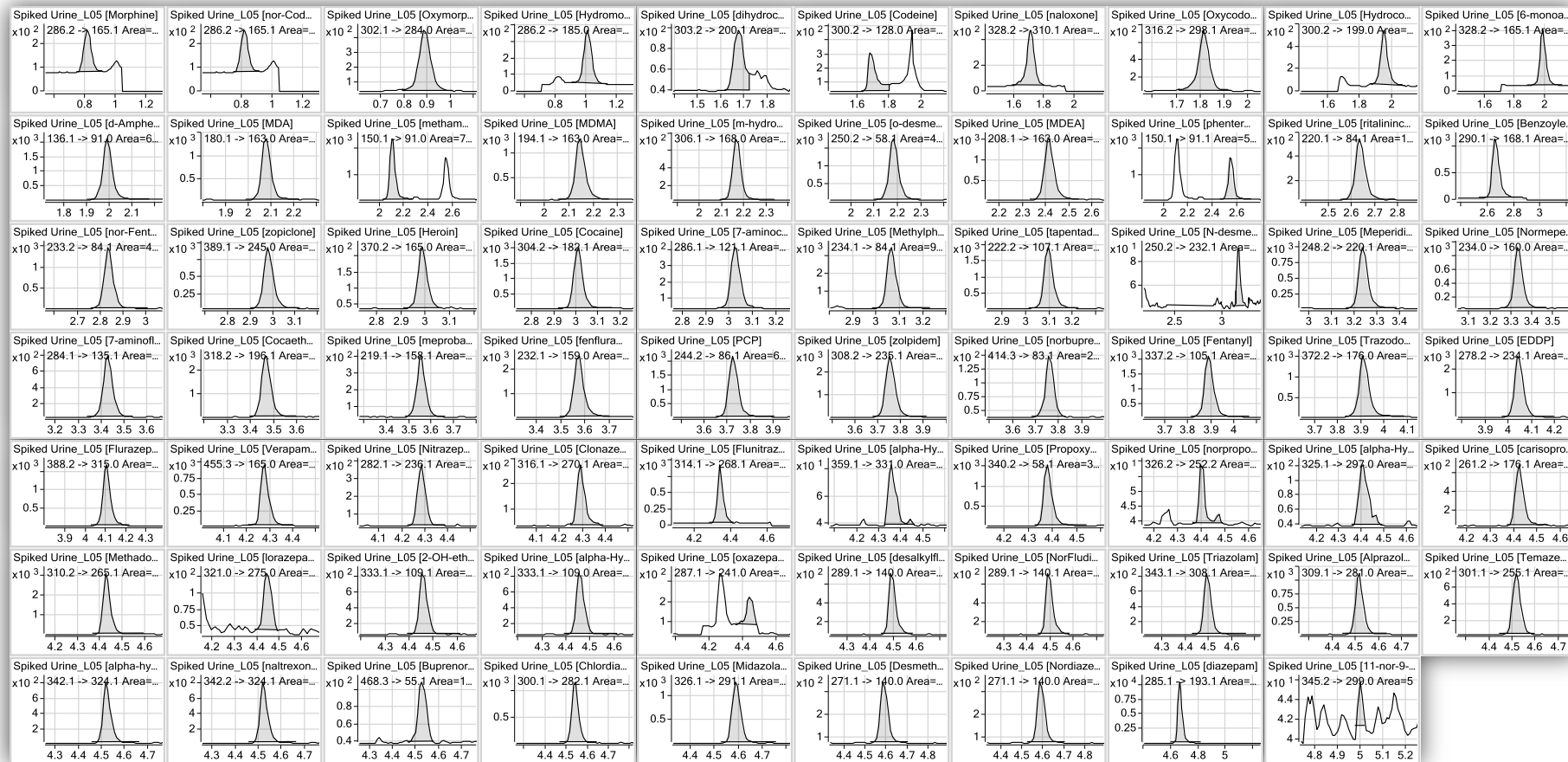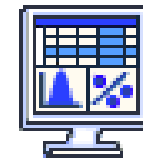
Quantitative Analysis
Batch at a Glance

Data Review with Compounds at a Glance
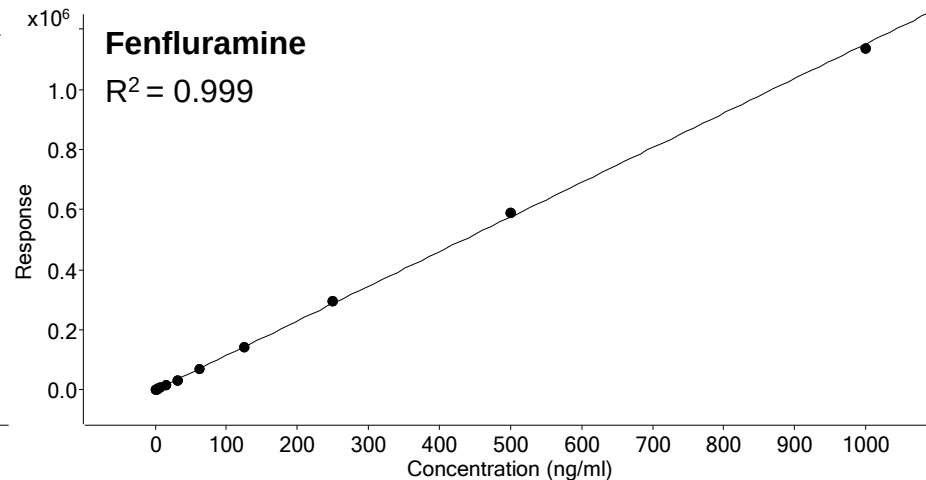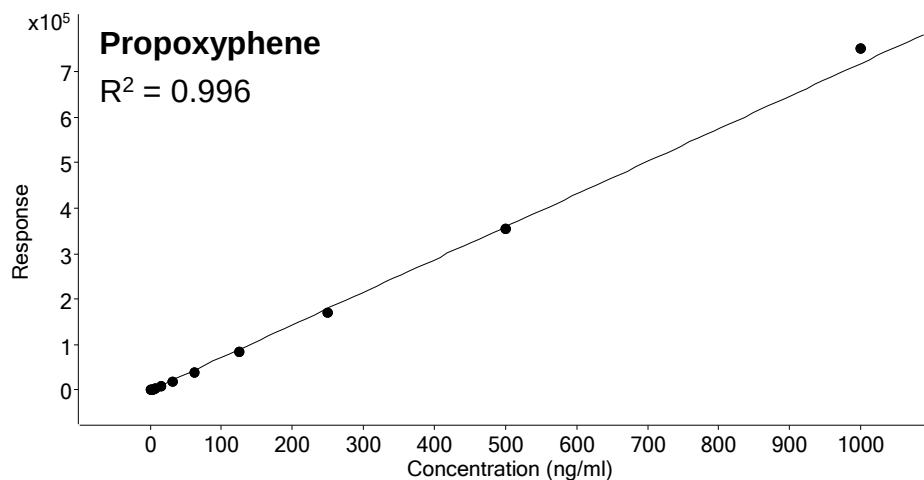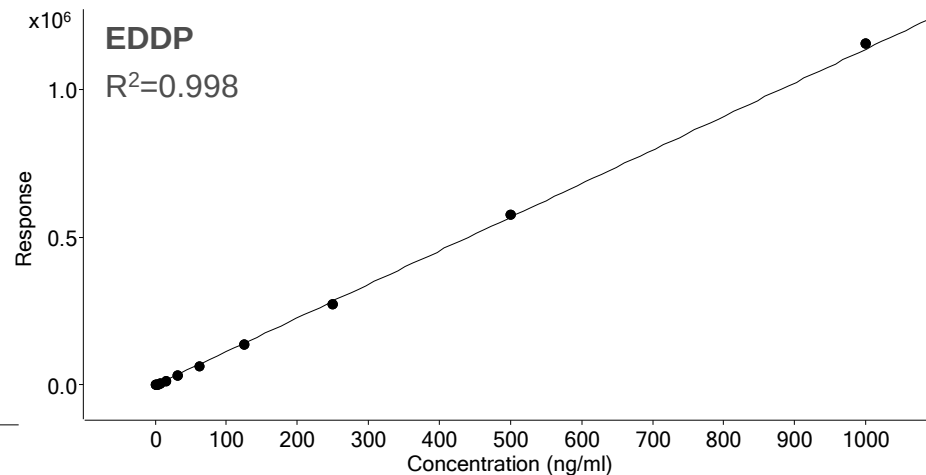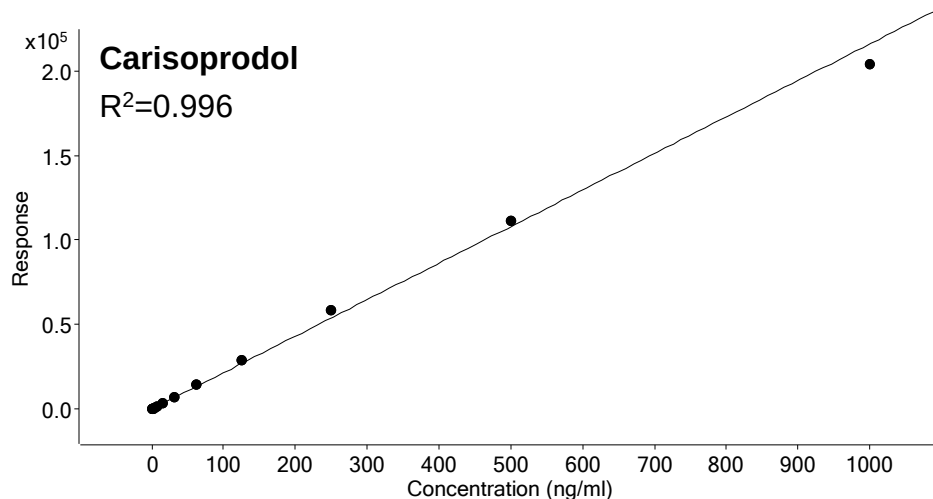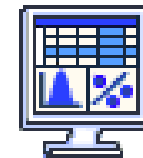
Quantative Analysis
Calibration Curves

Carisoprodol
R^2=0.996

EDDP
R^2=0.998

Propoxyphene
R^2 = 0.996

Fenfluramine
R^2 = 0.999

Customizable Reporting

Conclusions

- Agilent makes it easy to create custom analytical panels for the measurement of Opiates, Opioids, Benzodiazepines, Amphetamines & Illicits

- Panels can be comprehensive or focused to suit your needs

- Dynamic MRM functionality, automatic optimization and MRM transition Database help make method development straightforward

- Results can be achieved with a simple Dilute & Shoot sample preparation

- Agilent's MassHunter software is optimized for your data review and reporting workflow