

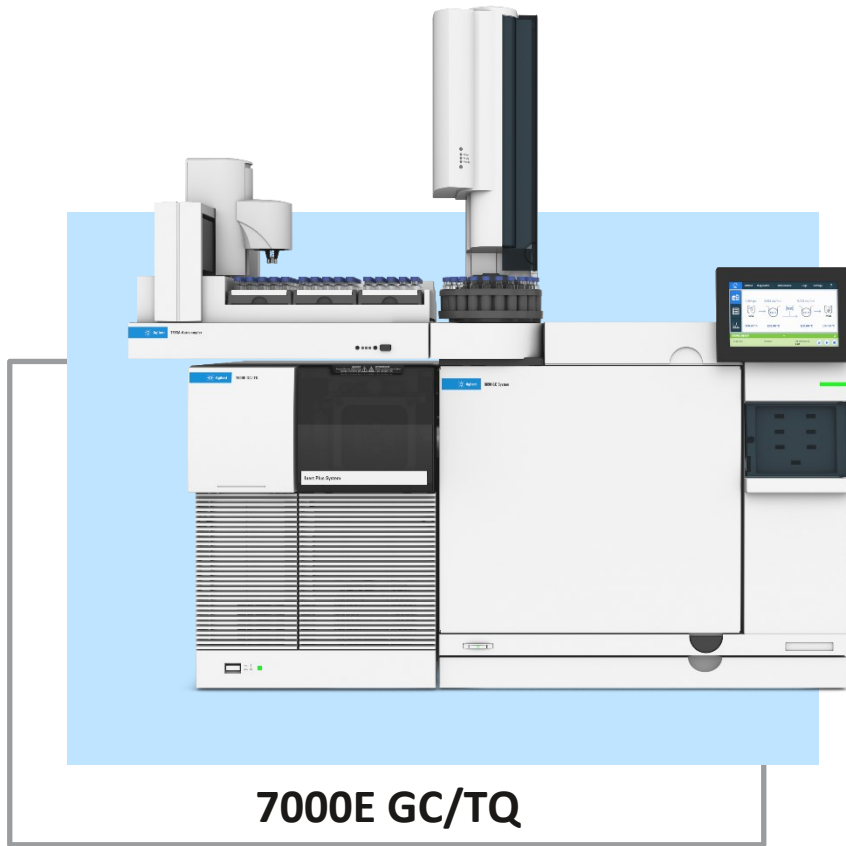
Agilent GC/MS QQQ 7010D: když jde citlivost s robustností ruku v ruce



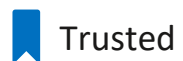
Altium

Jitka Zrostlíková

Agilent GC/MS trojité kvadrupóly



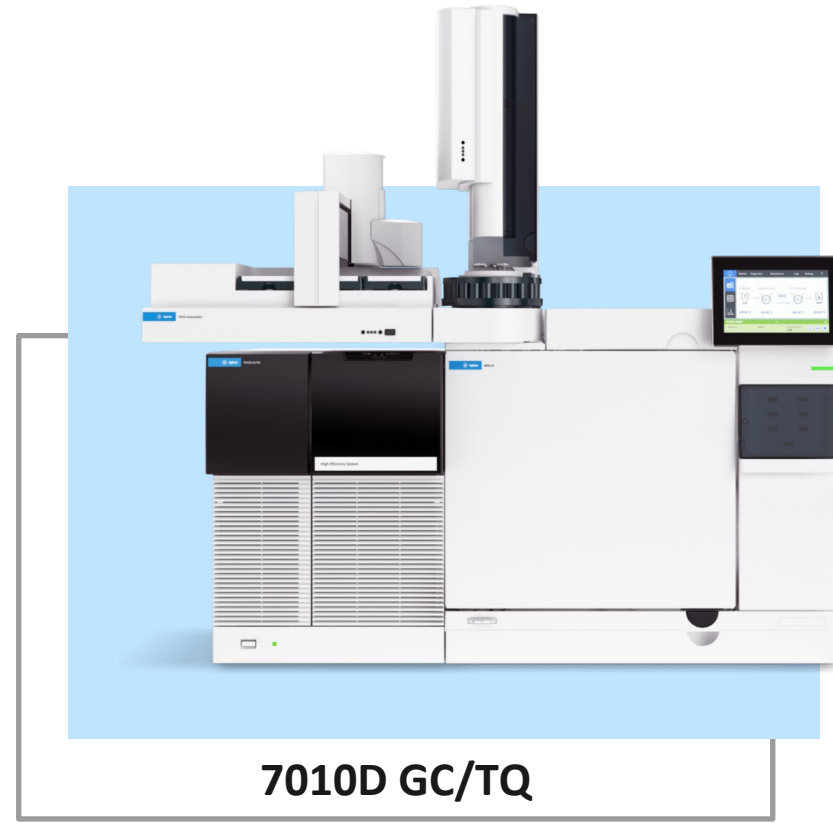
Rutinní výkonný systém



Versatility



Numerous Apps.



Ultra stopová analýza



Sensitivity



Specifications



Stability

Agilent 7010D GC/MS trojitý kvadrupól



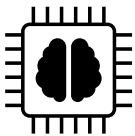
Hardware

Iontový zdroj HES 2.0
Excelentní citlivost a vysoká odolnost zátěži
matricí



Přístrojová intelligence

Chytré alerty, upozornění na údržby, SWARM
ladění, inteligentní GC



MassHunter 13

MRM optimizer, vylepšené RTL, Compliance

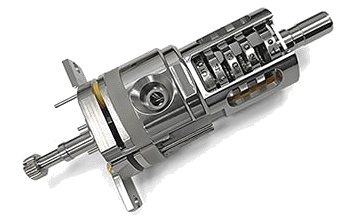




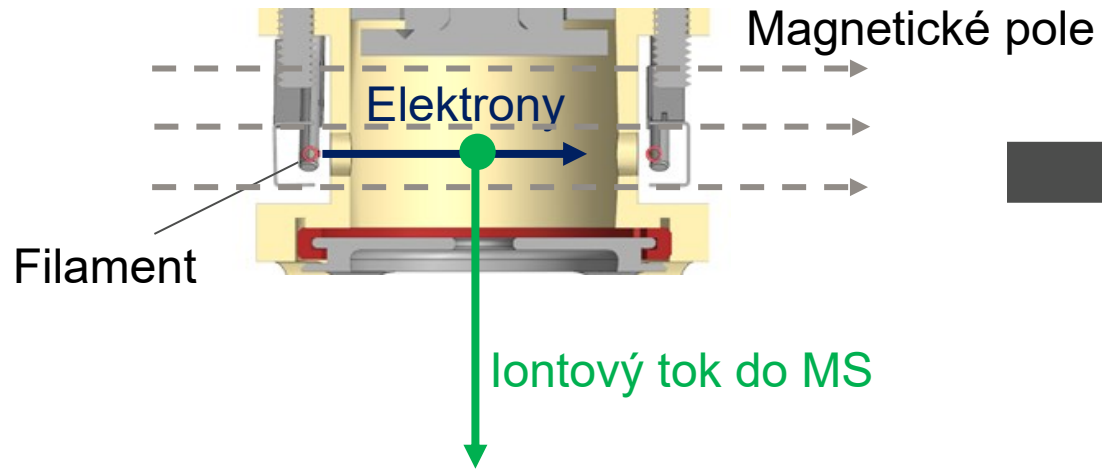
Altium

Hardware

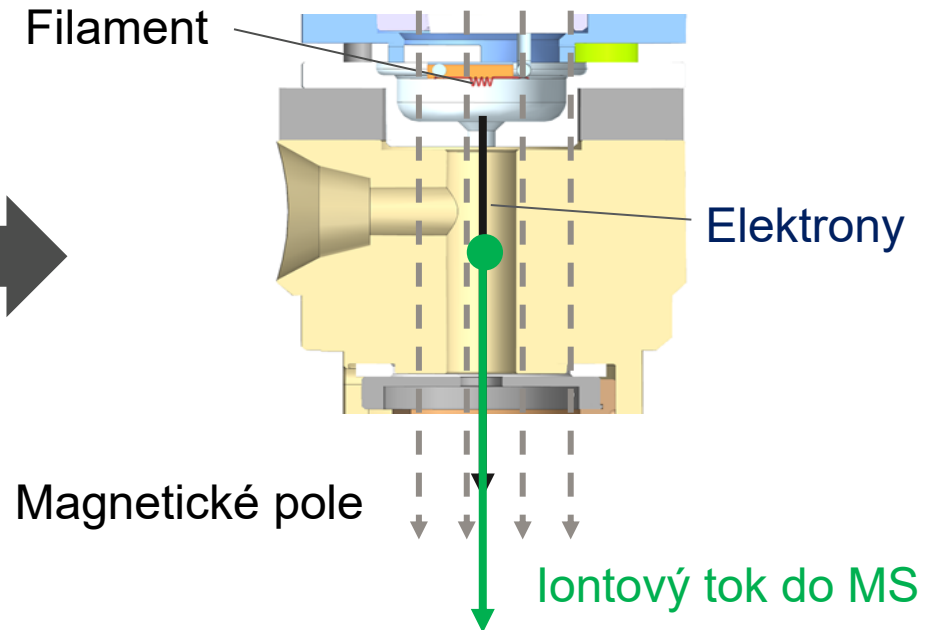
High efficiency source (HES)



Orthogonální iontový zdroj (Agilent Stainless Steel, Extractor, Hydrolnert)



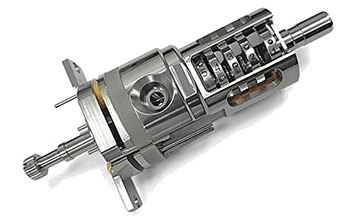
Axiální design (Agilent HES)



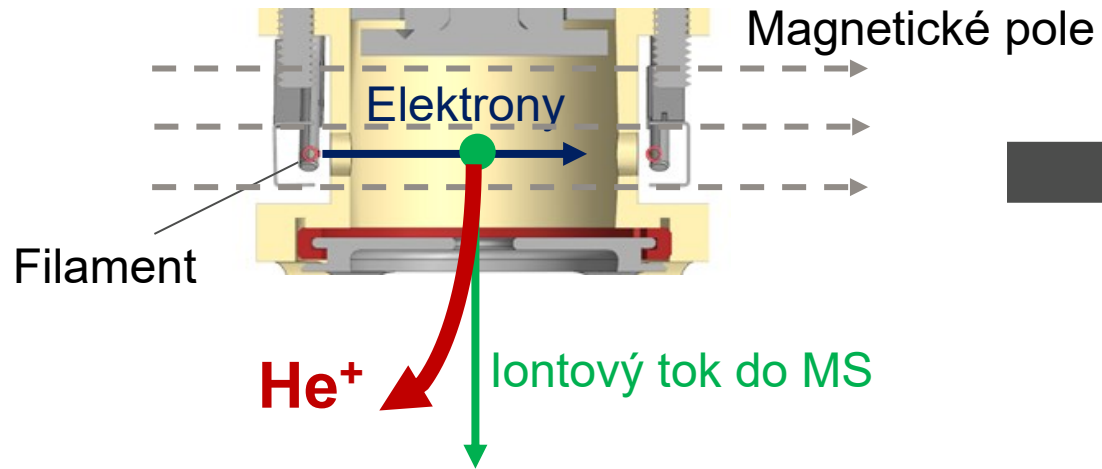
HES iontový zdroj: 10x vyšší signál analytů

- Nižší meze detekce
- Nižší množství vzorku = méně údržby

High efficiency source (HES)

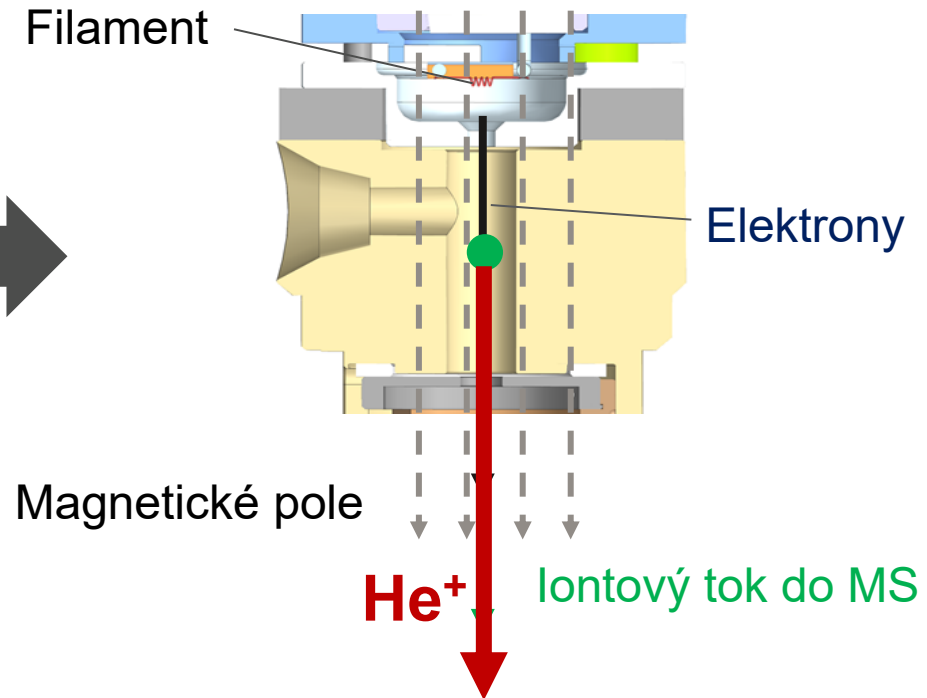


Orthogonální iontový zdroj (Agilent Stainless Steel, Extractor, Hydrolnert)



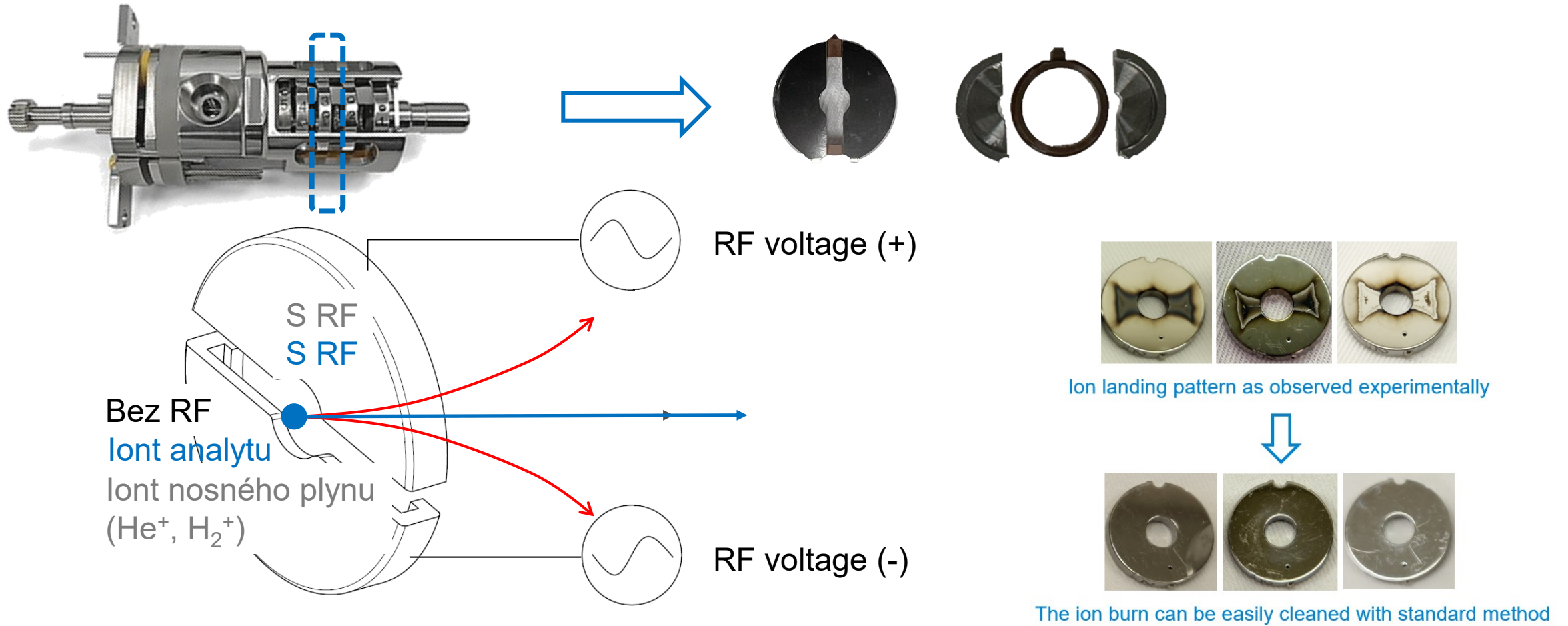
Velmi málo iontů nosného plynu vstupuje do kvadrupólu

Axiální design (Agilent HES)



Vysokoenergetické ionty nosného plynu vstupují do kvadrupólu

Nová generace iontového zdroje HES 2.0



Nově integrovaná čočka v iontovém zdroji **odklání malé ionty mimo osu** – minimalizace dopadu do kvadrupolu

Pod patentem US

Agilent 7010D Instrument Detection Limit (IDL)



7010A/B/C

Parameter	Value
EI MRM IDL	0.5 fg or less octafluoronaphthalene (OFN) Statistically derived at 99% confidence level from the area precision of eight sequential splitless injections* of 1 µL, 2 fg/µL OFN standard. MS/MS transition of m/z 272 → 222 100 msec dwell time

All tests were carried out on a 30 m × 0.25 mm, 0.25 µm column.
*IDL specification is only demonstrated if an autosampler is part of the installed system. If an autosampler is not present, the EI MRM S/N specification is performed.



7010D

Parameter	Value
EI MRM IDL	0.3 fg or less octafluoronaphthalene (OFN) Statistically derived at 99% confidence level from the area precision of eight sequential splitless injections* of 1 µL, 1 fg/µL OFN standard. MS/MS transition of m/z 272 → 222 100 msec dwell time

All tests were carried out on a 30 m × 0.25 mm, 0.25 µm column.
*IDL specification is only demonstrated if an autosampler is part of the installed system. If an autosampler is not present, the EI MRM S/N specification is performed.

Nižší chemický šum = lepší LOQ

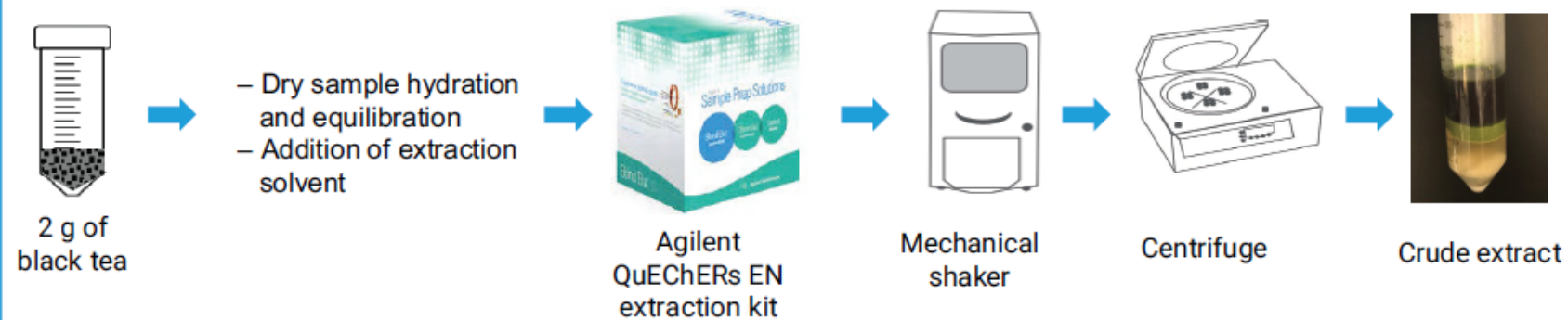
Důkaz místo slibů:
GC/MS/MS 7010D analýza
pesticidů v obtížné matrici

Metoda pro 246 pesticidů v černém čaji

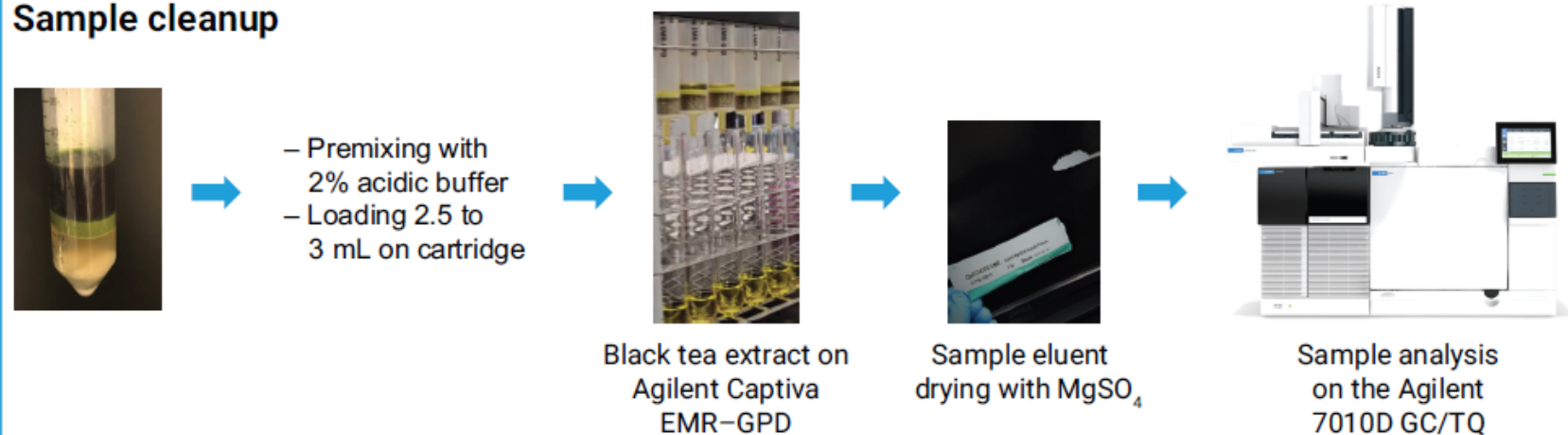
- **QuEChERS** extrakce z 2 g čaje, přečištění extraktu, celkem **5 x ředění**
- GC systém s využitím technologií **mid-column backflush** a **MMI cold splitless** nástřík
- GC/QQQ MS **Agilent 7000D** s HES 2.0 iontovým zdrojem
- Sběr dat v **dynamickém MRM** (dMRM) režimu – celkem **749 MRM přechodů**, až **64 konkurenčních** přechodů
- **Retention time locking (RTL)** během sběru dat
- Využití MRM databáze Agilent MassHunter **Pesticides and Environmental Pollutants 4.0** s retenčními časy
- Validace metody dle **SANTE 11312/2021 guideline**
- Testování **dlouhodobé stability systému > 800 nástříků** matričních vzorků

Příprava vzorku QuEChERS s přečištěním na Captiva EMR GPD

Sample extraction



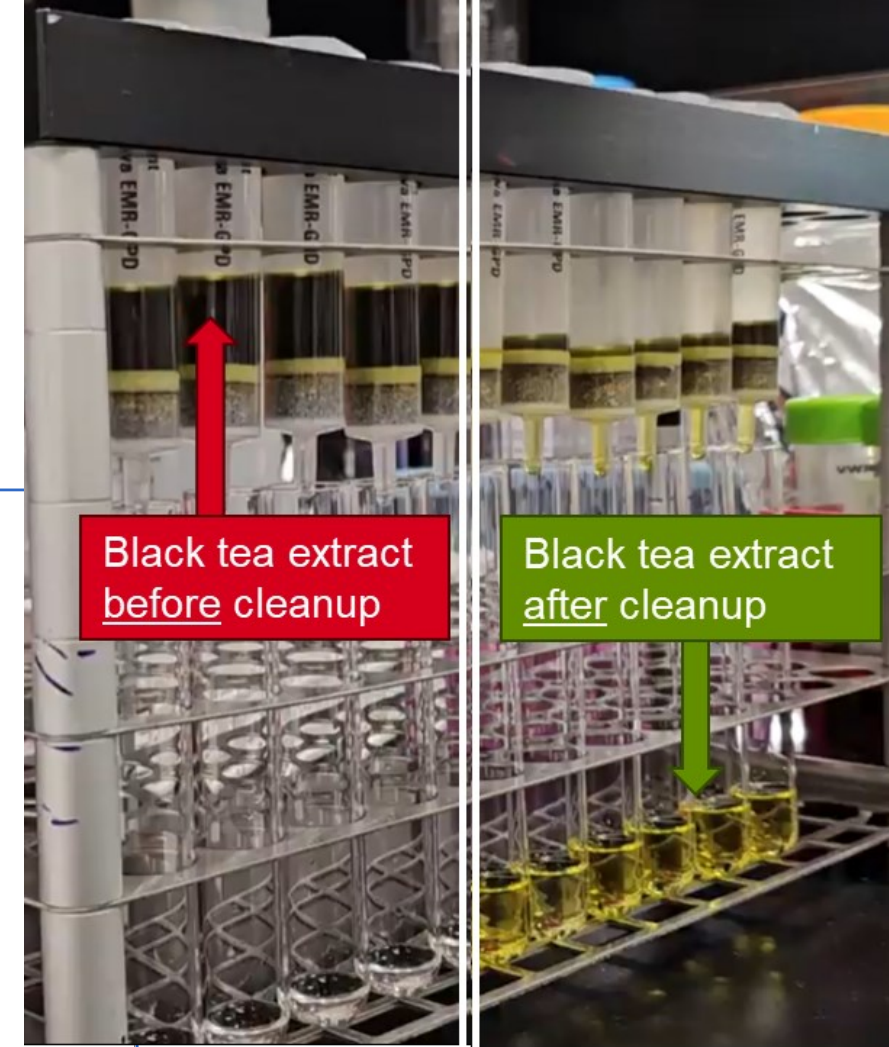
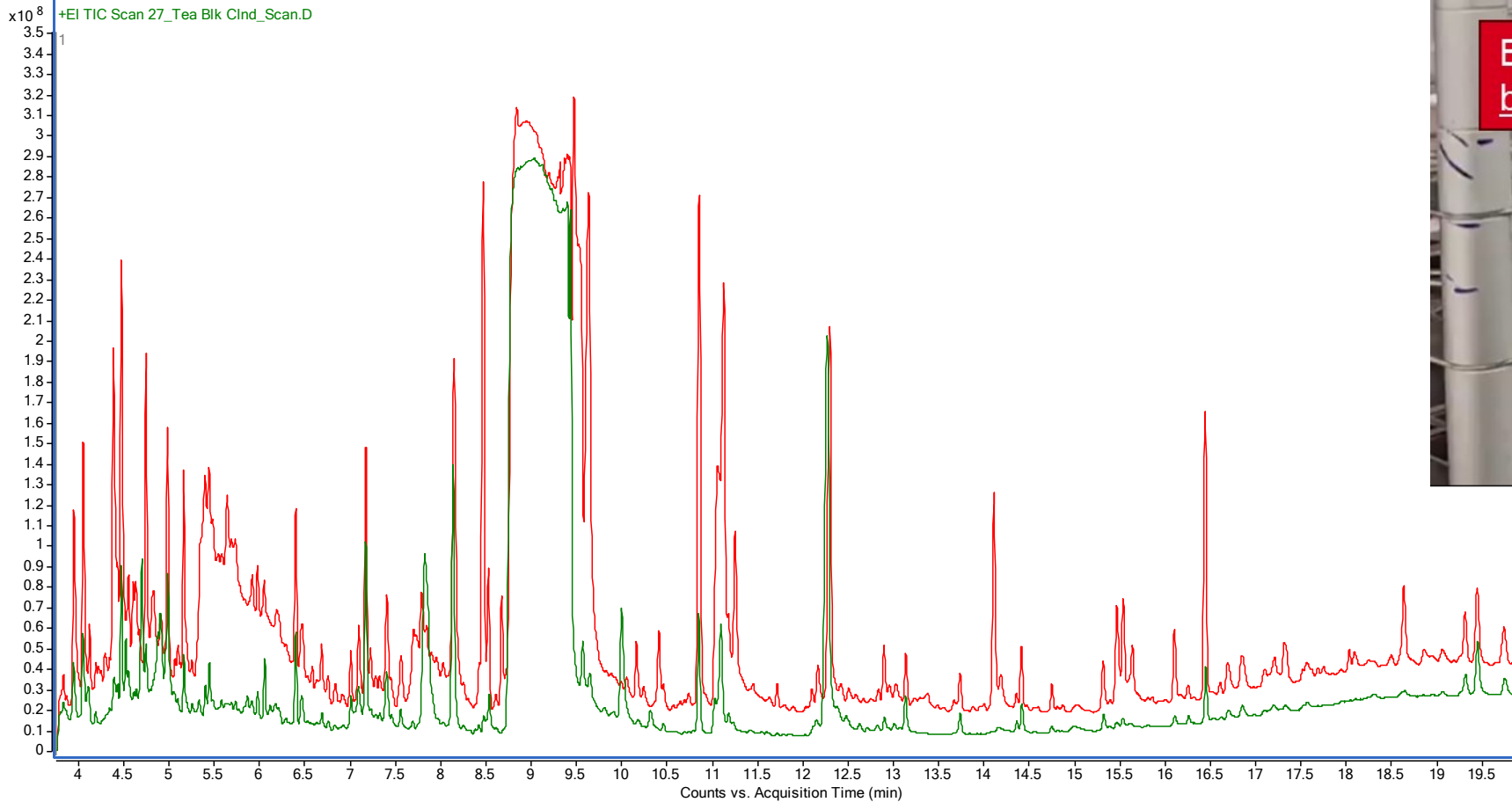
Sample cleanup



Příprava vzorku

Přečištění vzorků pomocí Captiva EMR-GPD*

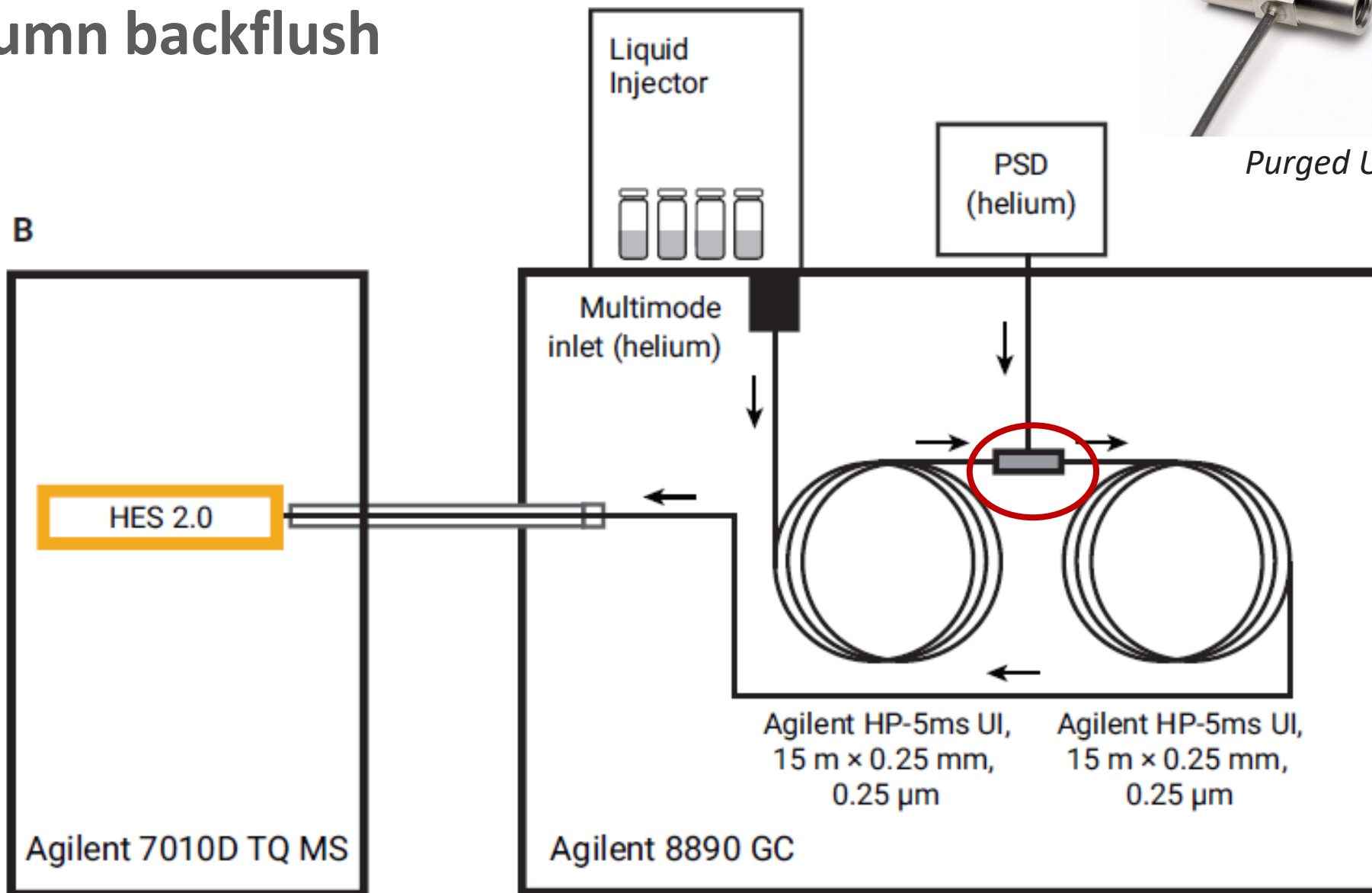
Chromatogram pozadí ve skenu (full MS)



*General Pigmented Dry

Konfigurace GC

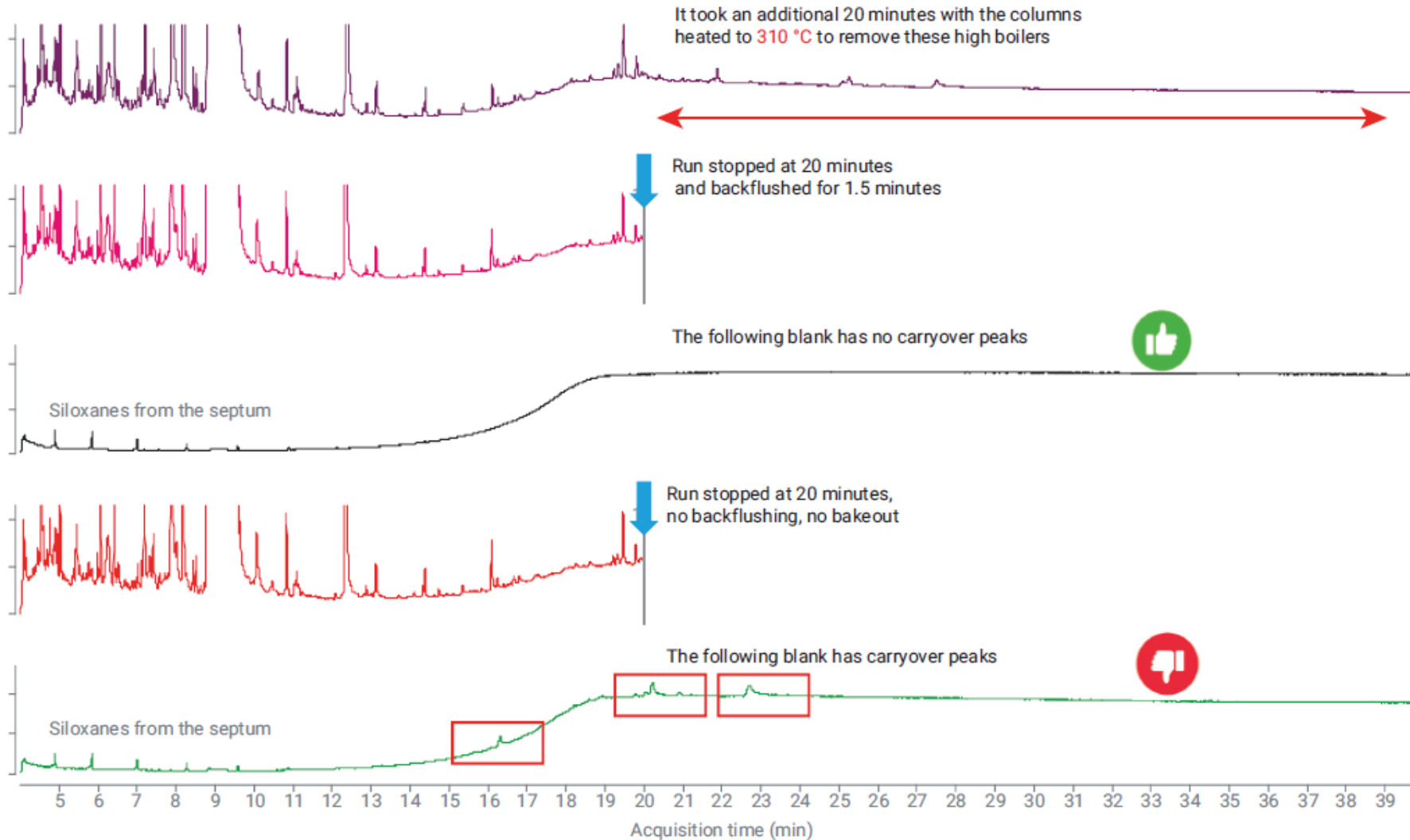
Mid-column backflush



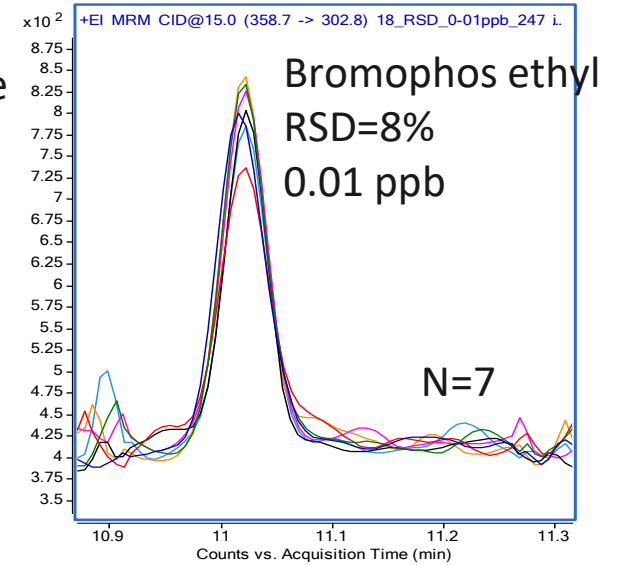
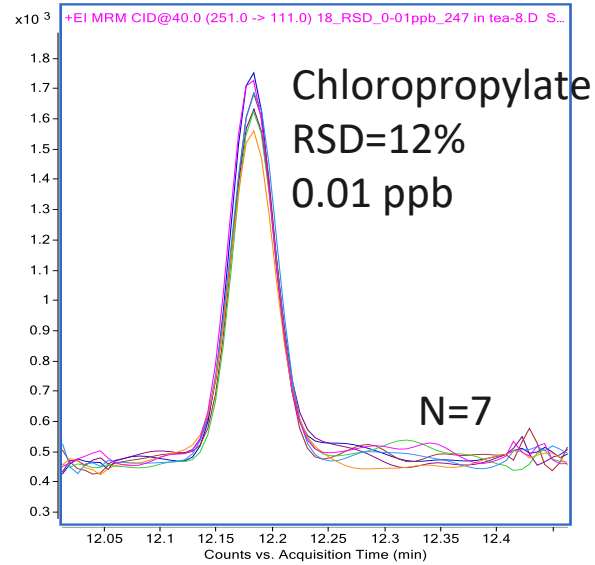
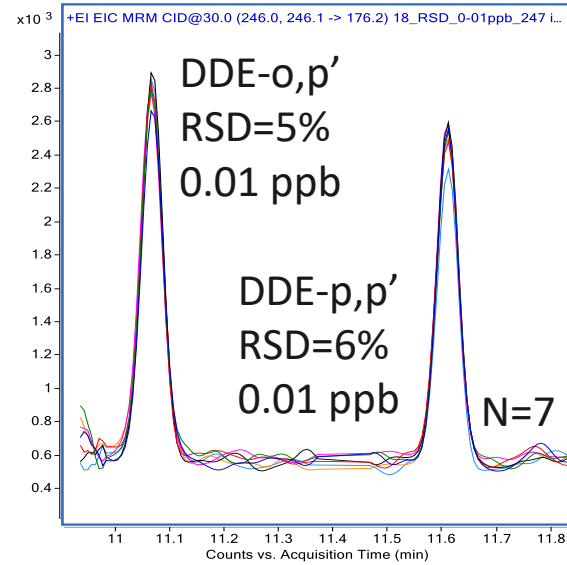
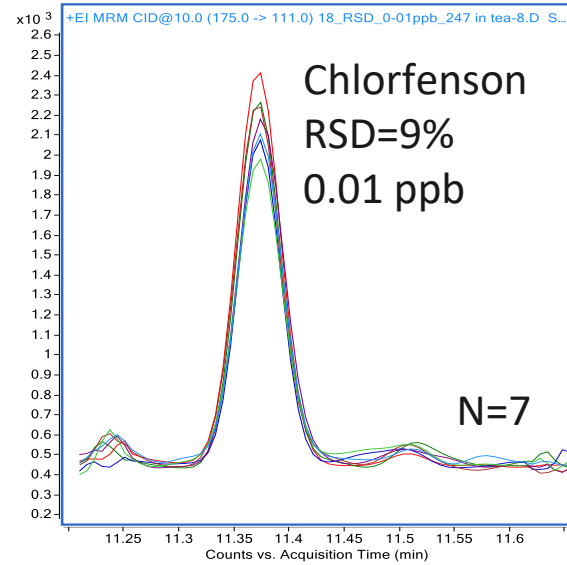
Purged Ultimate Union

Mid-column backflush

Možnost zkrácení metody a eliminace carryover



Výsledky validace: LOQ, linearita



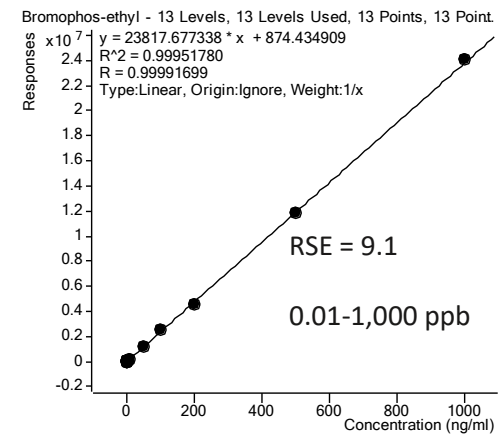
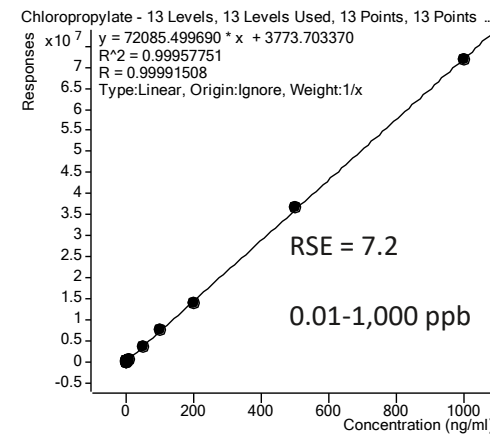
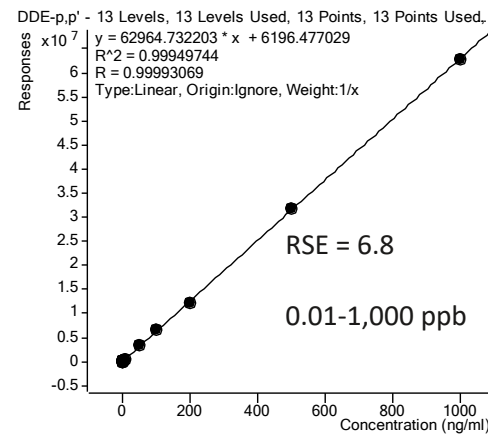
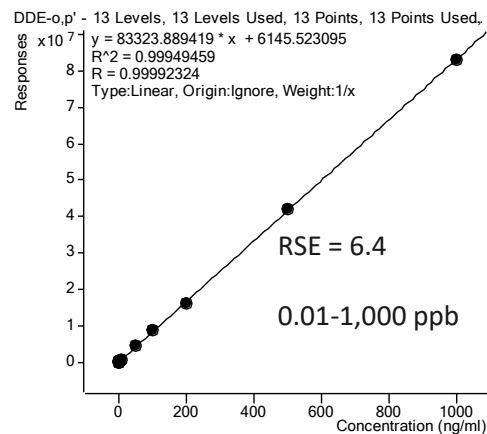
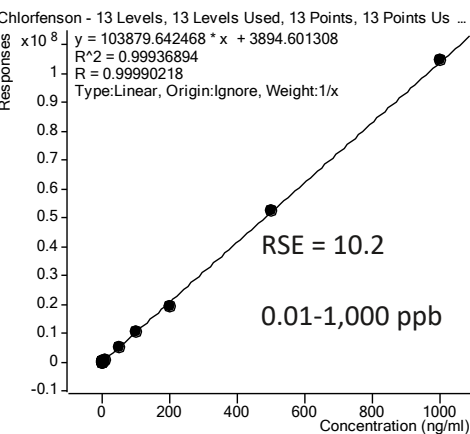
Chlorfenson

DDE-o,p'

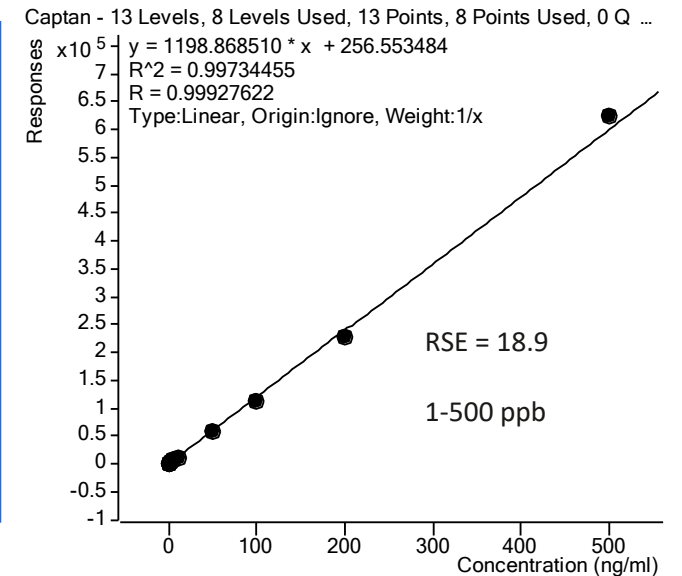
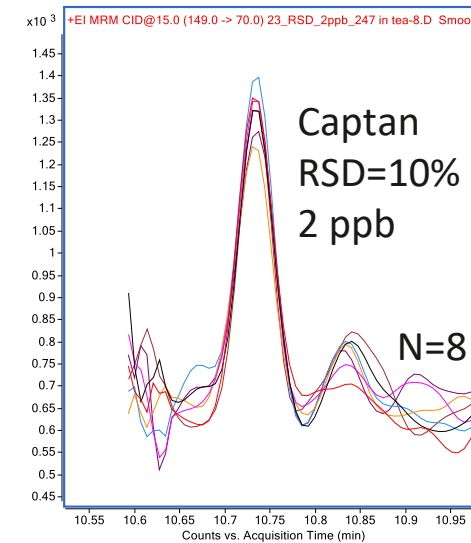
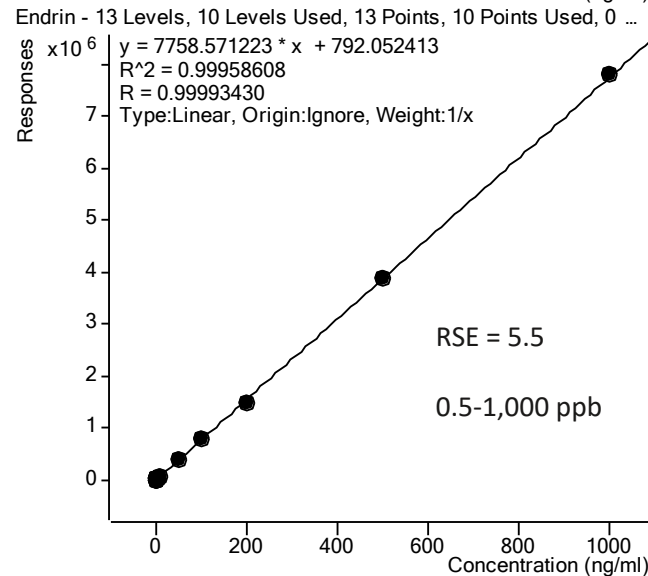
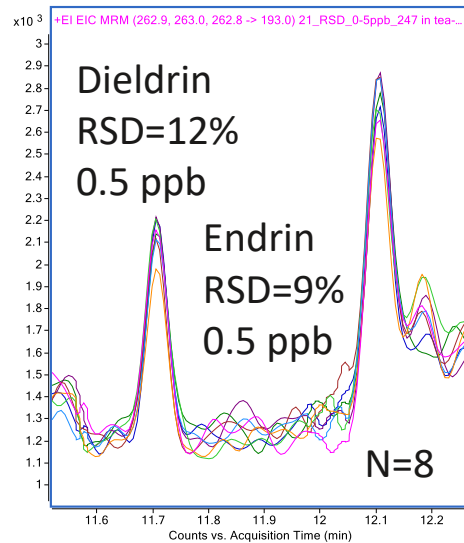
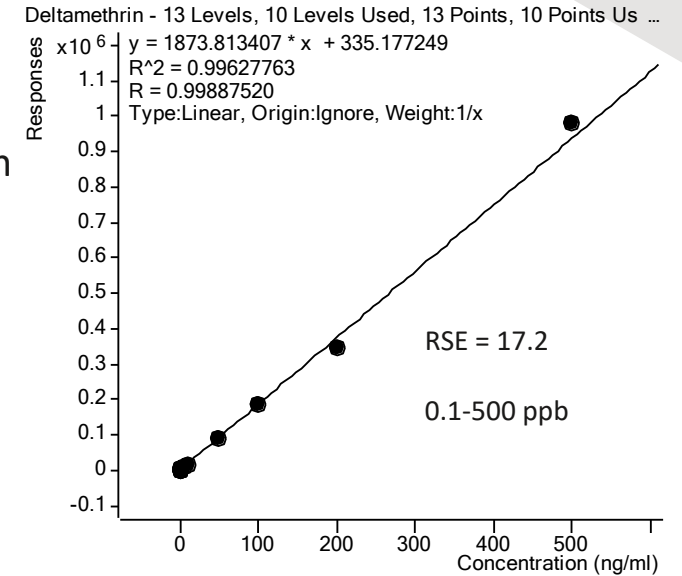
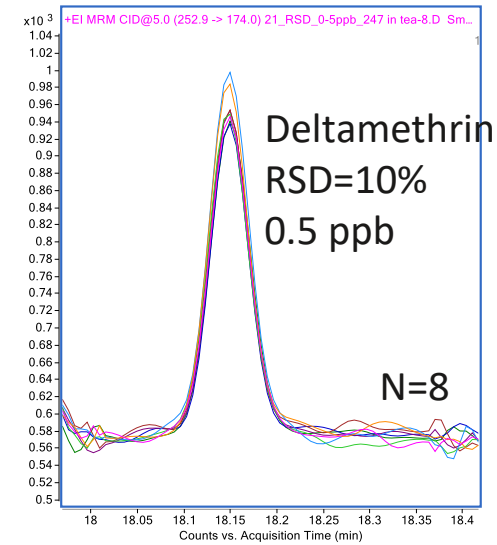
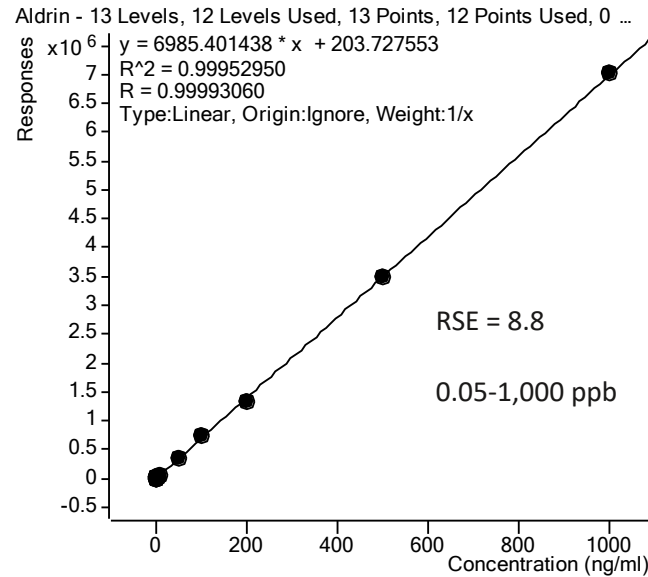
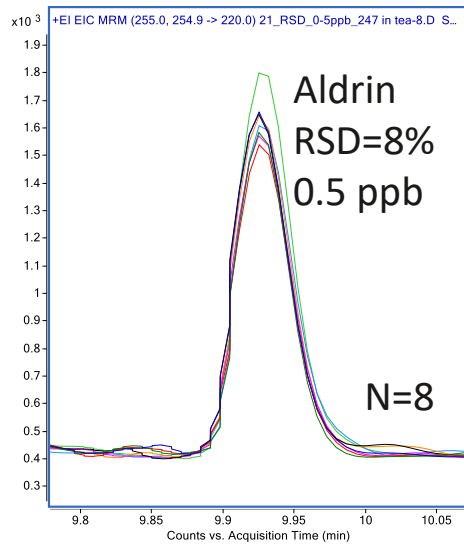
DDE-p,p'

Chloropropylate

Bromophos ethyl

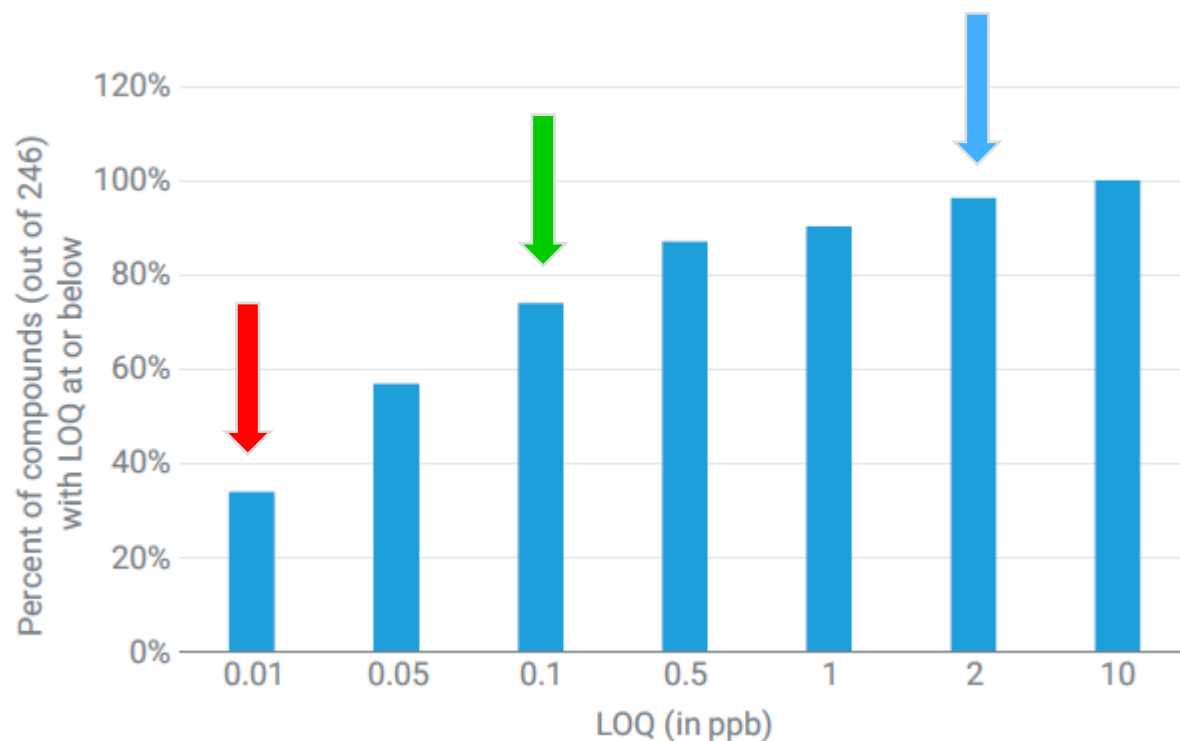


Výsledky validace: LOQ, linearita



Výsledky validace: LOQ, linearita

Histogram LOQ 246 pesticidů

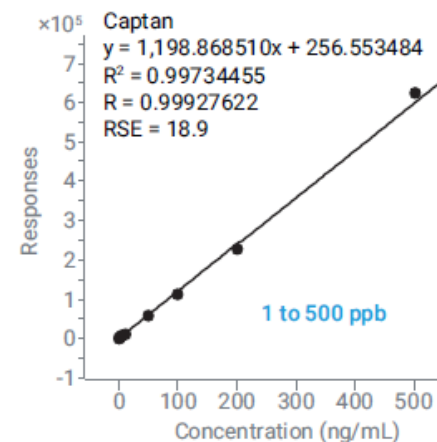
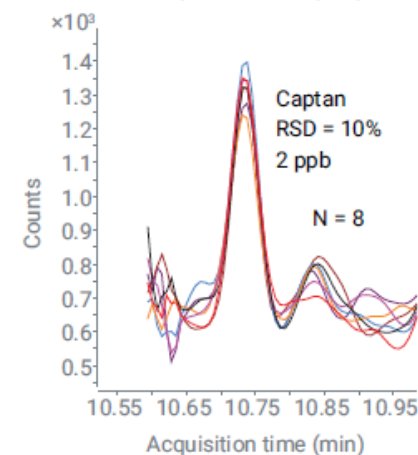
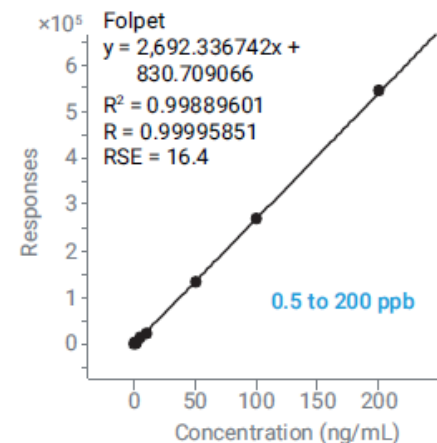
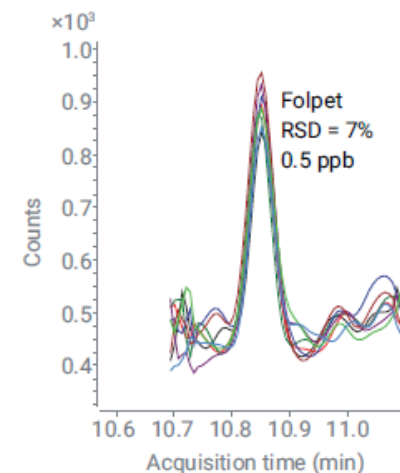


34% látek LOQ < 0,01 ppb

74% látek LOQ < 0,1 ppb

96% látek LOQ < 2 ppb

Captan a folpet



Dlouhodobá stabilita: 800 nástříků

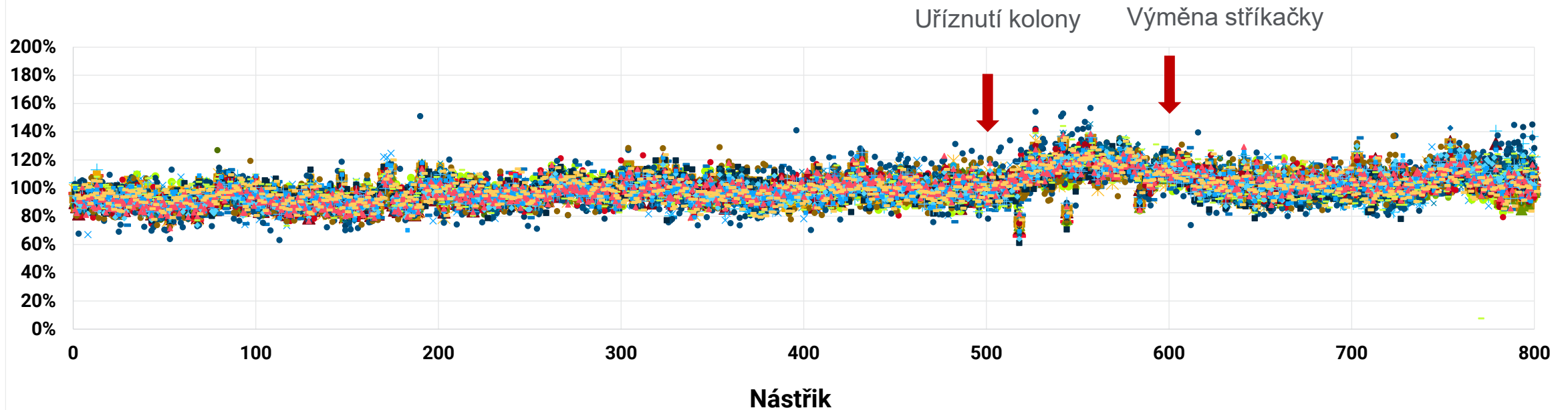
Podmínky experimentu:

- Extrakt čaje s přidavkem pesticidů na **úrovni 2 ppb**
- Každých **100 nástříků výměna lineru a septa** (< 4 min)
- Každých **500 nástříků uříznutí 5 cm kolony** (5-10 min)
- Po **600 nástřících** výměna stříkačky (5 min)
- **Žádné čištění** GC Inletu nebo MS detektoru

Dlouhodobá stabilita: 800 nástřiků

2 ppb pesticidy v černém čaji

Plochy normalizované na vnitřní standard (parathion-d10) a na průměrnou odezvu každého analytu



Brewing Excellence: Quantitating Over 200 Pesticides in Black Tea with Steady Performance and Maximized Uptime by GC/MS/MS



Authors

Anastasia A. Andrianova and
Limian Zhao
Agilent Technologies, Inc.

Abstract

This application note presents results for the sensitive and robust quantitation of 246 pesticides in black tea extract with the **Agilent 7010D Triple Quadrupole Mass Spectrometer** (GC/TQ) featuring a second-generation High Efficiency Source 2.0 (HES 2.0), that addresses the challenges posed by residual pesticide analysis in complex matrices. By optimizing sample preparation and using state-of-the-art GC/MS hardware, including ion source technology and midcolumn backflushing, excellent calibration performance and sensitivity at low-ppb levels were achieved. The method demonstrated exceptional ruggedness and robustness over 800 consecutive injections of a black tea extract spiked with pesticides at 2 ppb, with high precision and low RSDs, ensuring prolonged instrument uptime and maximum throughput. The demonstrated limits of quantitation (LOQs) were as low as 0.01 ppb for over a third of evaluated compounds, and the calibration range spanned up to five orders of magnitude while meeting SANTE 11312/2021 guidelines.

This application note highlights intelligent GC/TQ features, such as early maintenance feedback and an instrument health status dashboard, maintaining confidence in the results for a high-throughput analysis. The updated data acquisition platform provides enhanced user experience, including a new implementation of the retention time locking functionality.

Enhanced Longevity and Revolutionized Robustness for the Sensitive Detection of 190 Pesticides over 800 Injections



Author

Brooke C. Reaser
Agilent Technologies, Inc.

Abstract

Multiresidue pesticide analysis has become one of the most difficult but important analytical challenges for those using gas chromatography and mass spectrometry. The Agilent 8890 gas chromatograph (GC) coupled with the Agilent 7010 triple quadrupole mass spectrometer (GC/TQ) with a high efficiency source 2.0 (HES 2.0) upgrade is an analytically accurate, robust, and reproducible instrument for multiresidue pesticide analysis of complex samples. The analysis of 190 pesticides in a spinach extract was conducted using an Agilent QuEChERS extraction kit across 800 injections. Only GC inlet maintenance was required over the duration of the injections. The instrument configuration that enabled robust performance included a multimode inlet, a mid-column backflushing configuration, and the HES 2.0. No degradation of the analytical method, sensitivity, or instrument performance occurred, allowing for the high-throughput, accurate, robust, and sensitive detection of pesticides in spinach.



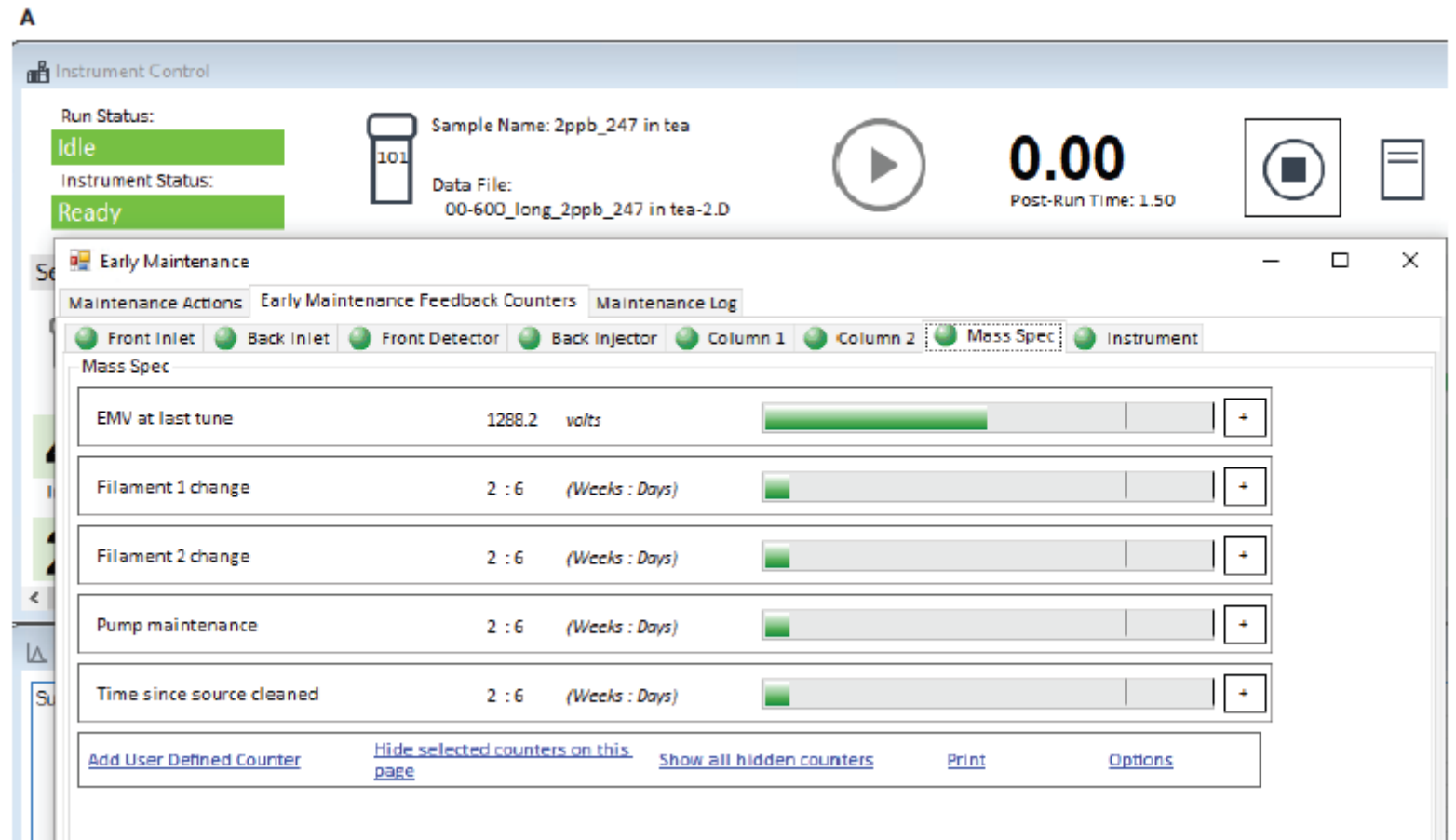
Altium

Přístrojová inteligence

Přístrojová inteligence

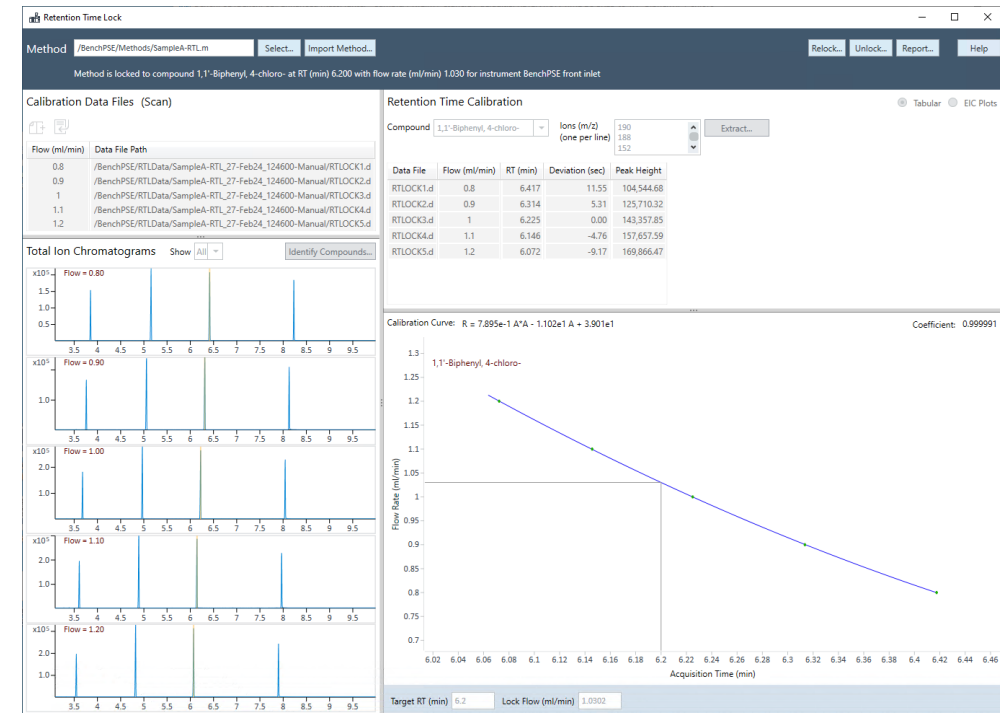
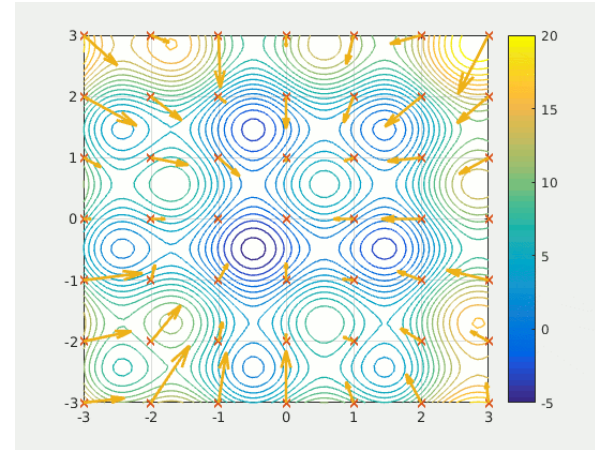
- **Včasné upozornění na údržby a chytrá upozornění**

Monitoruje „zdraví“ GC/MS přístroje a e-mailem zasílá upozornění na nutnou údržbu a zastavení chodu přístroje



Přístrojová inteligence

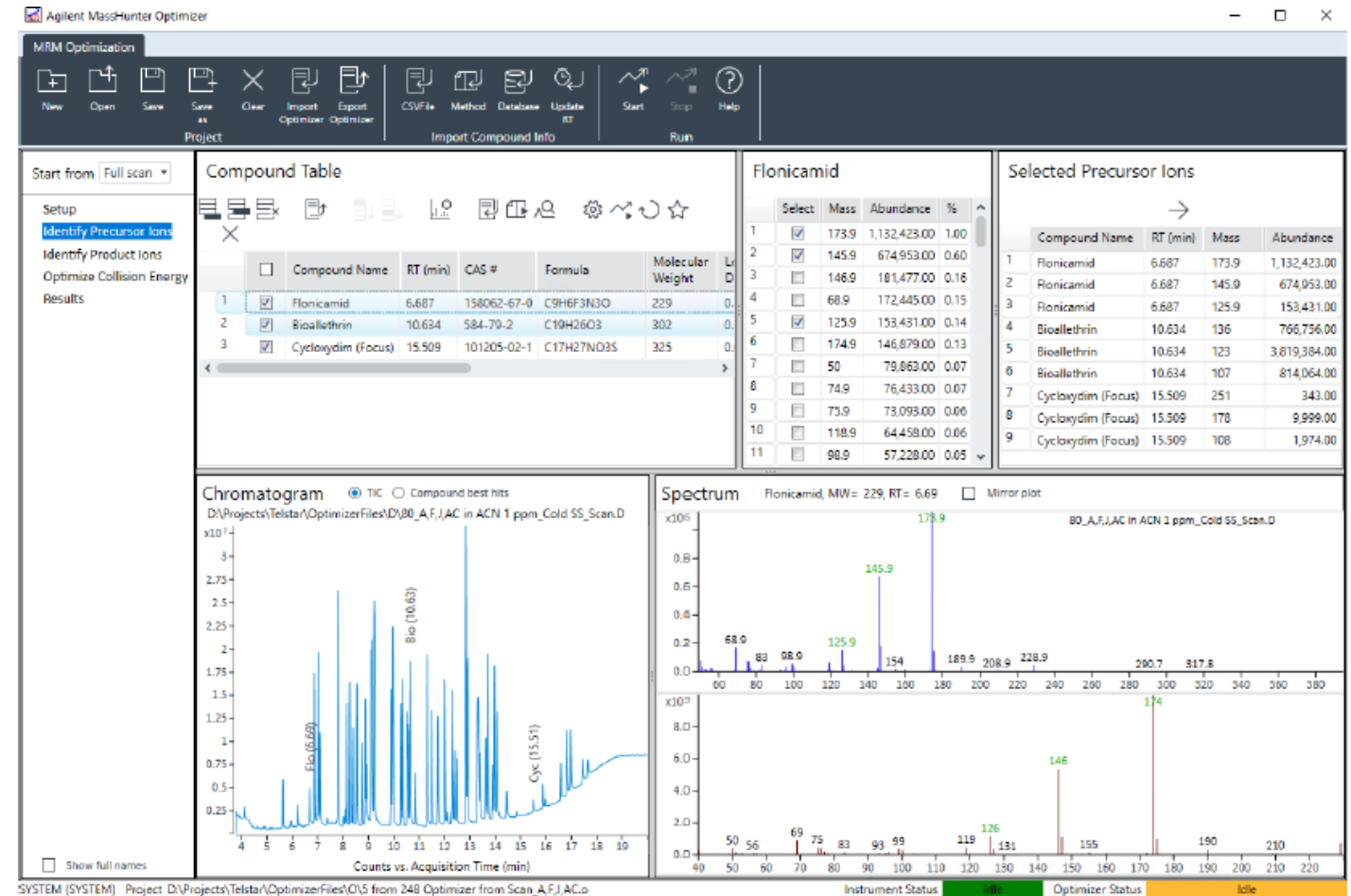
- **SWARM** autotune
- **Leak check** v reálném čase
- **Nový RT locking**



Přístrojová inteligence

■ Optimizer MRM přechodů

- ✓ Plná automatizace
- ✓ Zabudovaný přímo v akvizici
- ✓ Splňuje požadavky na „compliance“
- ✓ Jednoduchý transfer GC/MSD metody na GC/MS/MS metodu



Easy sample prep in MassHunter 13

Dvě věže



Easy sample prep in MassHunter 13

Blackbird {Blackbird}/Enhanced MassHunter - Test_Sample_Prep_01.M / atunes230.eiex.jtu

Method

Instrument

Sequence

Optimizer

Inlet/Injection Types...

View Data File Audit Trail

Edit Sample Prep...

Resource Library...

Edit Monitors...

Resource Layout...

GC Show/Hide Status

Reset Resources...

Instrument Options

Sample Prep

Instrument Control

Run Status:

Idle

Instrument Status:

Not Ready

Sample Name: Test_Blank_01

Data File: Test_A_plus_istd_noscan08.D

Sequence

Method (GC ALS)

36

72

1.1

Oven Temperature

Inlet-F Temperature

Column-1 Flow Calc.

Resource Layout

Import Layout

Export Layout

Layout Print Preview

Resource Library

Help

Tray Resources

Wash/Waste Vial Assignment

Resource Name:

Resource Type: Chemical Resource

Use Type: ☒ By Volume ☐ By Use

Usable Volume per Vial (µL): 1500

Uses per Vial: 1

Display Color: CadetBlue

Default Syringe Parameters

For Syringe Size (µL):

Wash Volume (µL):

Pump Volume (µL):

Draw Speed (µL/min): 1

Dispense Speed (µL/min): 1

Draw Needle Depth Offset (mm): -2.0

Use Needle Depth Offset for Dispense: ☐

Viscosity Delay (s): 0

Air Gap (% Syringe Size):

Overfill (% Syringe Size):

Layout Comment:

Vial Range:

Add

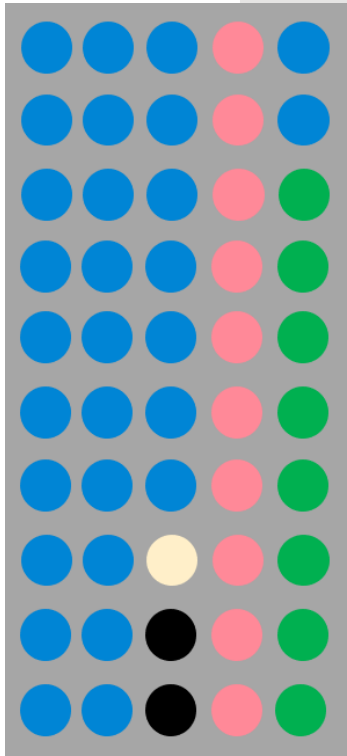
Remove

Replace

Cancel

Color	Name	Resource Type	Vial Range	Usage
Green	Solvent Vials - IsoOctane	Chemical Resource	11-20	1700 µL
Pink	Ethyl Benzene d10 - ISTD	Chemical Resource	23	1400 µL
Black	100 ppm Sample A	Chemical Resource	21	400 µL
Yellow	10 ppm Sample A	Chemical Resource	22	700 µL

Save Layout



- Empty Vial
- Solvent Vial
- Stock Vial
- ISTD Vial
- Unoccupied

Správa dat a uživatelů, systémy
pro regulované prostředí

Požadavky na zabezpečení kvality dat v regulovaném prostředí



Energy



Chemical



Environment



Food



Pharmaceuticals
& Supplements



Forensics

Technical Control	Executive order	ISO 17025	40 CFR Part 80, 160	ISO 17025	21 CFR Part 11	CAP
Ochrana dat	●	●	●	●	●	●
Kontrola přístupových oprávnění	●	●	●	●	●	●
Audit Trail		●	●	●	●	●
E-Signature				●	●	●
Vestavěný reporting	●	●	●	●	●	●

OpenLab řídicí panel

MANAGEMENT

 Edit Instrument

 Delete Instrument

 Refresh All

 Edit Privileges

 Lock Instrument

 Configure Instrument

 Show Instrument Files

 Create Acquisition Desktop Shortcuts

 Update GC Firmware

 Update MS Firmware

 Create QTOF TuneCond Desktop Shortcut

 Copy to Clipboard

Instruments and Locations

Properties

Actions

Selected Row

Instruments

Instruments

Location A

5975_7890

5977C

5977C_8890

7890B Only

8890 Only

Ana Elsa

Arsine

BenchPSE

Chandler

DESKTOP-9CKQSH3

GC only

MODI_8890

PorkyPig_CCrossans

TQ SC4

Instruments

Projects

Administration

BenchPSE

Idle

Project: BenchPSE

Launch

Launch Offline

Status

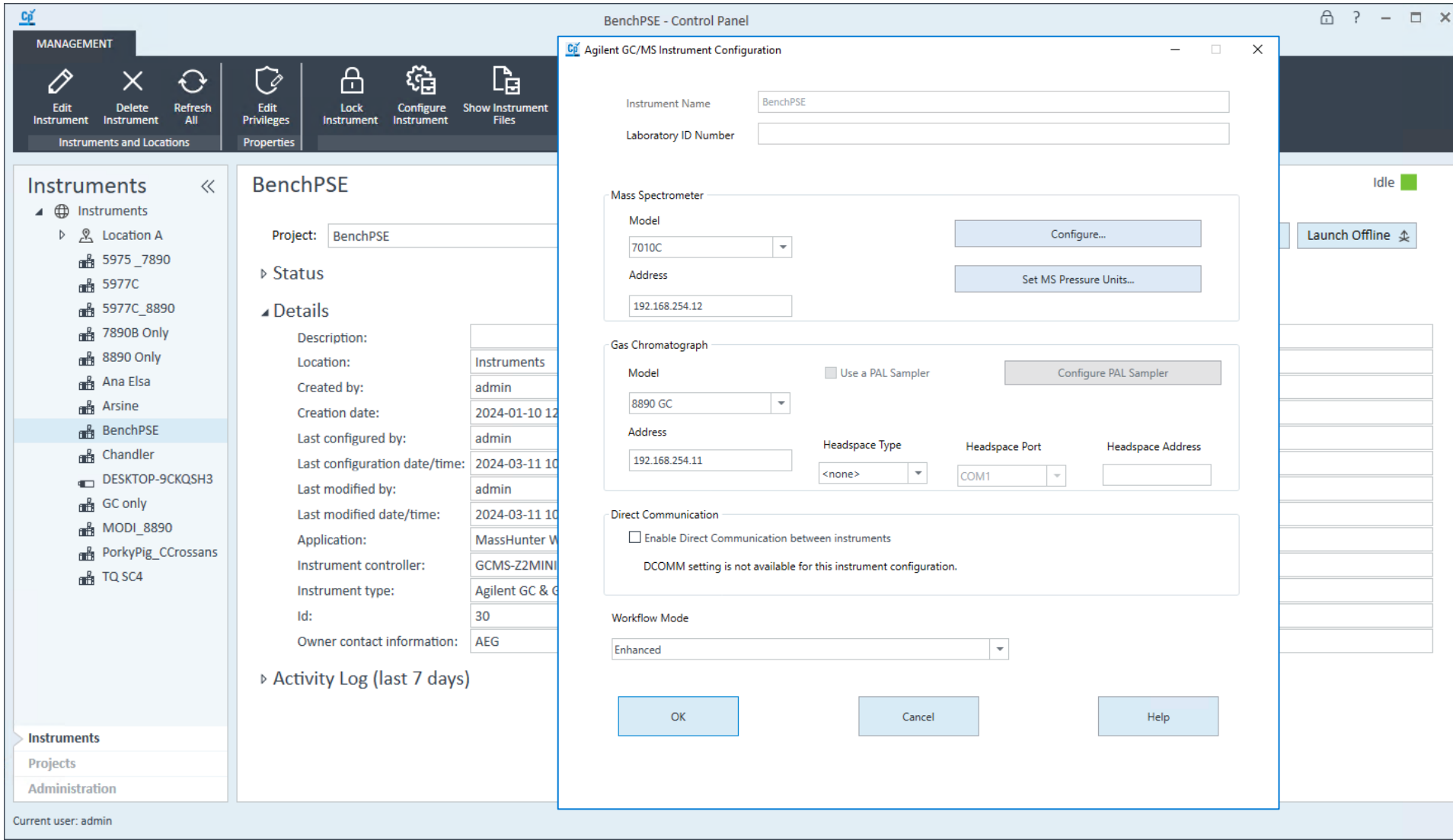
Details

Description:	
Location:	Instruments
Created by:	admin
Creation date:	2024-01-10 12:30:51-08:00
Last configured by:	admin
Last configuration date/time:	2024-03-11 10:18:59-07:00
Last modified by:	admin
Last modified date/time:	2024-03-11 10:18:59-07:00
Application:	MassHunter Workstation
Instrument controller:	GCMS-Z2MINI1
Instrument type:	Agilent GC & GCMS Systems
Id:	30
Owner contact information:	AEG

Activity Log (last 7 days)

Current user: admin

Konfigurace přístroje/přístrojů



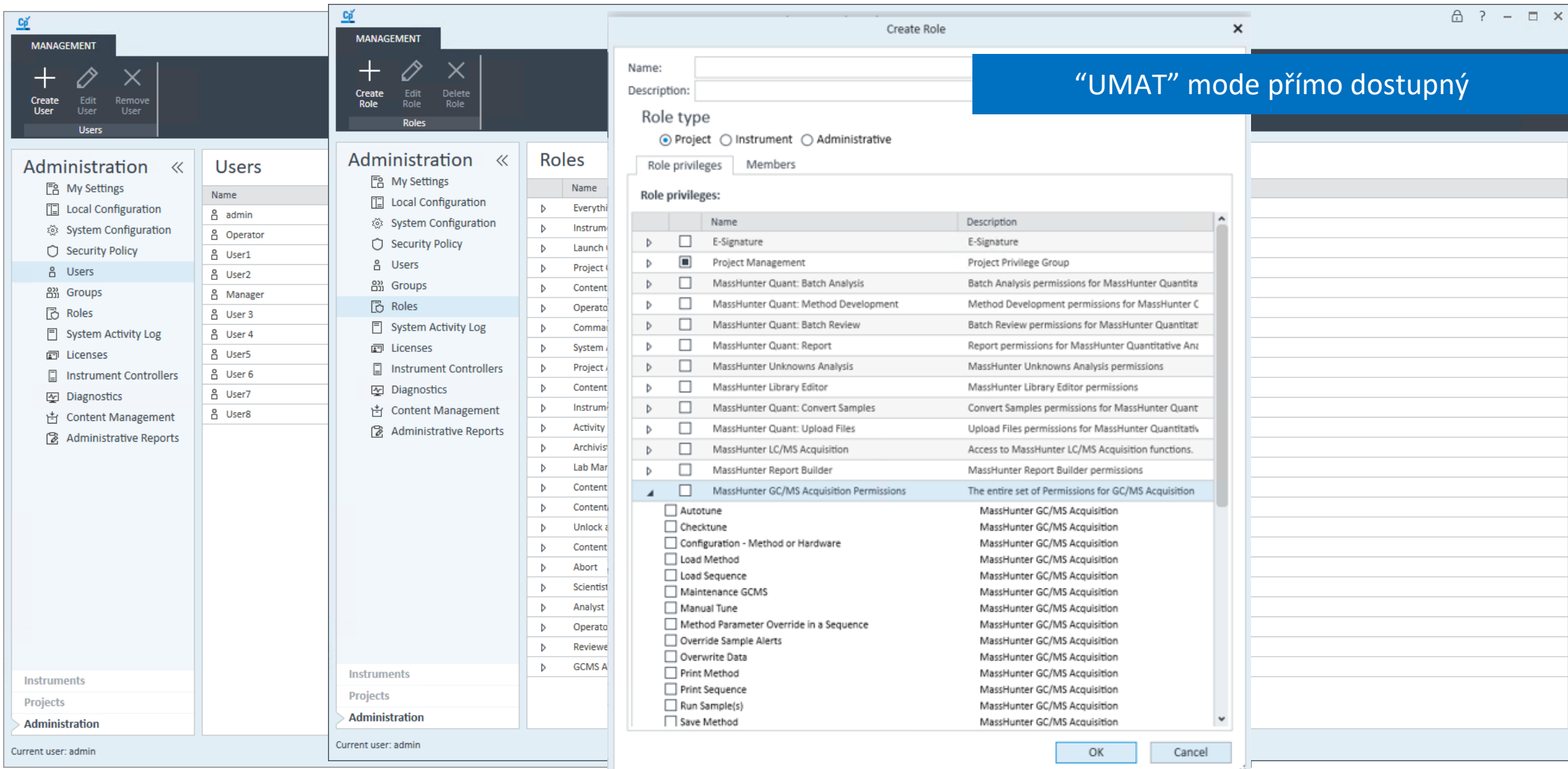
The screenshot displays the BenchPSE - Control Panel interface. On the left, a sidebar shows a list of instruments under the 'Instruments' section, with 'BenchPSE' selected. The main panel shows the 'BenchPSE' configuration details, including project name, status, and details like description, location, and creation date. A table lists the instrument's configuration details.

The 'Agilent GC/MS Instrument Configuration' dialog box is open, showing the following fields and options:

- Instrument Name:** BenchPSE
- Laboratory ID Number:** (empty)
- Mass Spectrometer:**
 - Model:** 7010C
 - Address:** 192.168.254.12
- Gas Chromatograph:**
 - Model:** 8890 GC
 - Address:** 192.168.254.11
 - Headspace Type:** <none>
 - Headspace Port:** COM1
 - Headspace Address:** (empty)
- Direct Communication:**
 - ☐ Enable Direct Communication between instruments
 - DCOMM setting is not available for this instrument configuration.
- Workflow Mode:** Enhanced

Buttons at the bottom of the dialog include OK, Cancel, and Help.

Uživatelské role a oprávnění



The screenshot displays the Altium NEXUS user management interface. The main window shows the 'Users' and 'Roles' sections. The 'Roles' section is active, and the 'Create Role' dialog box is open. The dialog box has a 'Name' field, a 'Description' field, and a 'Role type' section with three radio buttons: 'Project' (selected), 'Instrument', and 'Administrative'. Below the 'Role type' section are two tabs: 'Role privileges' and 'Members'. The 'Role privileges' tab is active, showing a list of permissions. A blue callout box highlights the 'UMAT' mode as directly accessible.

MANAGEMENT

Users

Administration

- My Settings
- Local Configuration
- System Configuration
- Security Policy
- Users**
- Groups
- Roles
- System Activity Log
- Licenses
- Instrument Controllers
- Diagnostics
- Content Management
- Administrative Reports

Users

Name
admin
Operator
User1
User2
Manager
User 3
User 4
User5
User 6
User7
User8

MANAGEMENT

Roles

Administration

- My Settings
- Local Configuration
- System Configuration
- Security Policy
- Users
- Groups
- Roles**
- System Activity Log
- Licenses
- Instrument Controllers
- Diagnostics
- Content Management
- Administrative Reports

Roles

Name
Everything
Instrument
Launch
Project
Content
Operator
Comm
System
Project
Content
Instrument
Activity
Archiv
Lab Mar
Content
Content
Unlock
Content
Abort
Scientist
Analyst
Operator
Review
GCMS A

Create Role

Name:

Description:

Role type

☒ Project ☐ Instrument ☐ Administrative

Role privileges **Members**

Role privileges:

	Name	Description
☐	E-Signature	E-Signature
☒	Project Management	Project Privilege Group
☐	MassHunter Quant: Batch Analysis	Batch Analysis permissions for MassHunter Quantita
☐	MassHunter Quant: Method Development	Method Development permissions for MassHunter C
☐	MassHunter Quant: Batch Review	Batch Review permissions for MassHunter Quantitat
☐	MassHunter Quant: Report	Report permissions for MassHunter Quantitative An
☐	MassHunter Unknowns Analysis	MassHunter Unknowns Analysis permissions
☐	MassHunter Library Editor	MassHunter Library Editor permissions
☐	MassHunter Quant: Convert Samples	Convert Samples permissions for MassHunter Quant
☐	MassHunter Quant: Upload Files	Upload Files permissions for MassHunter Quantitativ
☐	MassHunter LC/MS Acquisition	Access to MassHunter LC/MS Acquisition functions.
☐	MassHunter Report Builder	MassHunter Report Builder permissions
☒	MassHunter GC/MS Acquisition Permissions	The entire set of Permissions for GC/MS Acquisition
☐	Autotune	MassHunter GC/MS Acquisition
☐	Checktune	MassHunter GC/MS Acquisition
☐	Configuration - Method or Hardware	MassHunter GC/MS Acquisition
☐	Load Method	MassHunter GC/MS Acquisition
☐	Load Sequence	MassHunter GC/MS Acquisition
☐	Maintenance GCMS	MassHunter GC/MS Acquisition
☐	Manual Tune	MassHunter GC/MS Acquisition
☐	Method Parameter Override in a Sequence	MassHunter GC/MS Acquisition
☐	Override Sample Alerts	MassHunter GC/MS Acquisition
☐	Overwrite Data	MassHunter GC/MS Acquisition
☐	Print Method	MassHunter GC/MS Acquisition
☐	Print Sequence	MassHunter GC/MS Acquisition
☐	Run Sample(s)	MassHunter GC/MS Acquisition
☐	Save Method	MassHunter GC/MS Acquisition

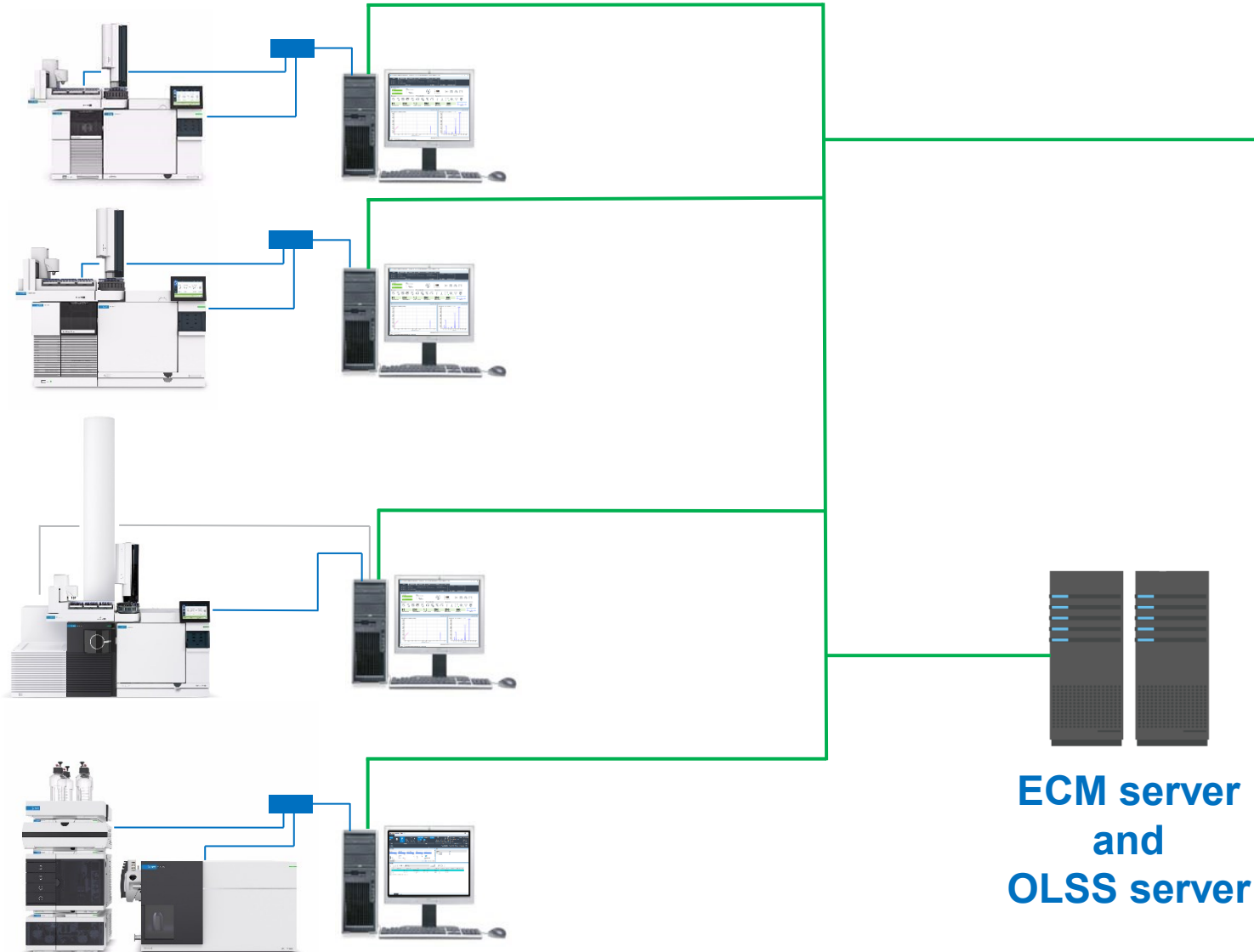
“UMAT” mode přímo dostupný

Current user: admin

Current user: admin

OK Cancel

Client/server řešení pro MassHunter systémy



Co si odnést domů...

Agilent 7010D a MassHunter 13

- ✓ Nový citlivější a robustnější GC/MS/MS s iontovým zdrojem HES 2.0
- ✓ **Přístrojová inteligence** a nové funkce: **MRM optimizer** a **RT locking** přímo v akvizici, **Easy sample prep**
- ✓ Možnost **nastavení uživatelských rolí a oprávnění**, **Client/server** management dat





Děkuji za
pozornost...