Applications of Field-Mobile Purge and Trap GC/MS for Onsite Water Analysis (and much more)

Garth Patterson

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FLIR Mass Spectrometry

- Founded 2001 as Griffin Analytical
- West Lafayette, IN
- 15,400 sq ft in Purdue Research Park
- 45 Employees, 75% Technical Staff
- Develop mass spec and associated products (GC, handheld samplers)
- Transitioned to ICxT in 2005
- ICxT joined FLIR systems in 2010
- FLIR MS is still located in the Purdue Research Park

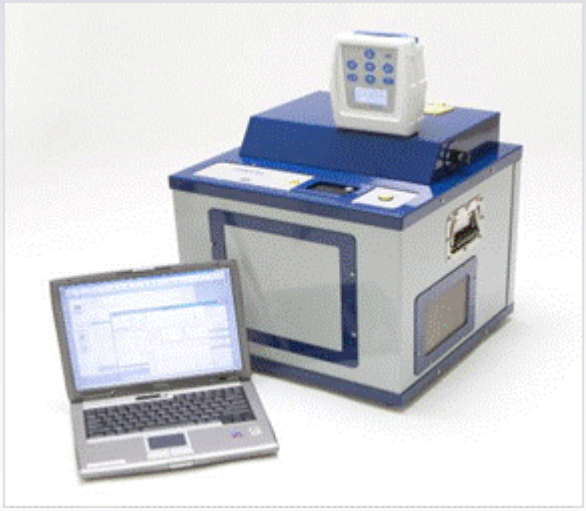
GRIFFIN | 450 – Mobile/Field-Ready GC/MS/MS

Overview and Specifications

- Gas Chromatograph/Mass Spectrometer
- Detects, Identifies, and Confirms ppt concentrations of CWA's, TICS/TIMS, explosives, and pesticides
- Ruggedized and shock mounted for mobile platform use
- Flexible sample inlets for varying end-user applications
- MS/MS capability

- Size ……..…….. 19.2" x 19.2" x 21.1"
- Weight ……..…....85 lbs
- Mass Range……..…425 amu / Unit Mass Resolution
- Power Requirement.....……115-220 VAC, 50/60 Hz

Griffin 450



Benefits

- DIRECT AIR ANALYSIS
  - Sample Loop and Pre-concentration
  - Compatible with Griffin X-Sorber
- Ease of Use
- Extended Analytical Flexibility
- Rapid Response Time
- Positive Identification of Known and Unknown Chemical Threats
- Low Operational/Sustainment Costs
- Minimal Training Required

Key Customers

- DoD Operations
- Public Transportation Facilities
- International Governments Labs
- Mobile Laboratory Applications
- Demil Facilities

FLIR

PREPLESS

PREP

PSI-PROBE
Vapor / Solid / Liquid
Narcotics, Law Enforcement

THERMAL DESORBER
Vapor
Fire Debris, Law Enforcement

PURGE & TRAP
Water
Groundwater, Enviro Remediation

DIRECT SAMPLING LINE
Vapor
Building Monitoring , 24/7 Security

SPME
Vapor / Liquid
Accidental Spill, Incident Response

PSI-PROBE
Vapor / Solid / Liquid
Narcotics, Law Enforcement

AUTOSAMPLER
Liquid / Solid
Research & Academia

SYRINGE
Liquid / Solid
Sensitive Site Exploitation, Field-based Forensics

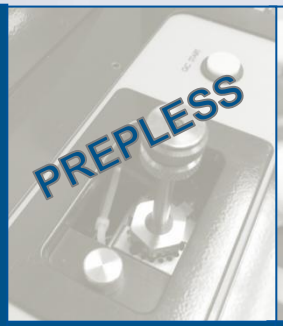
HEADSPACE
Liquid / Solid
Soil Contamination, Environmental Monitoring

Multi-Modal Sampling

Griffin 460

Griffin 400

Split/Splitless Injector for sampling via:



PSI Probe

SPME

PSI Probe

Syringe

Headspace

Autosampler

Griffin 460

Universal Sampling Port for sampling via:

X-Sorber

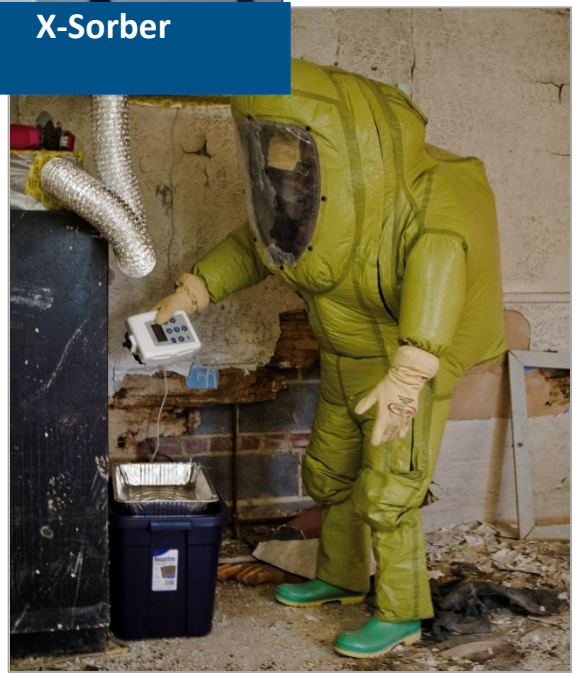
Purge & Trap

Sampling Line

GRIFFIN X-Sorber Accessory

- Air Samples
- First Smart, Handheld Remote Sampler
- Single button operation
- Deconable, Reusable
- GPS, sample metrics, and unattended operation
- Collects VOC's/SVOC's onto sorbent tubes
- GC/MS thermally desorbs sample from X-Sorber and performs identification of VOC's/SVOC's in sample
- ppb to ppt Detection

X-Sorber



GRIFFIN Purge & Trap Accessory

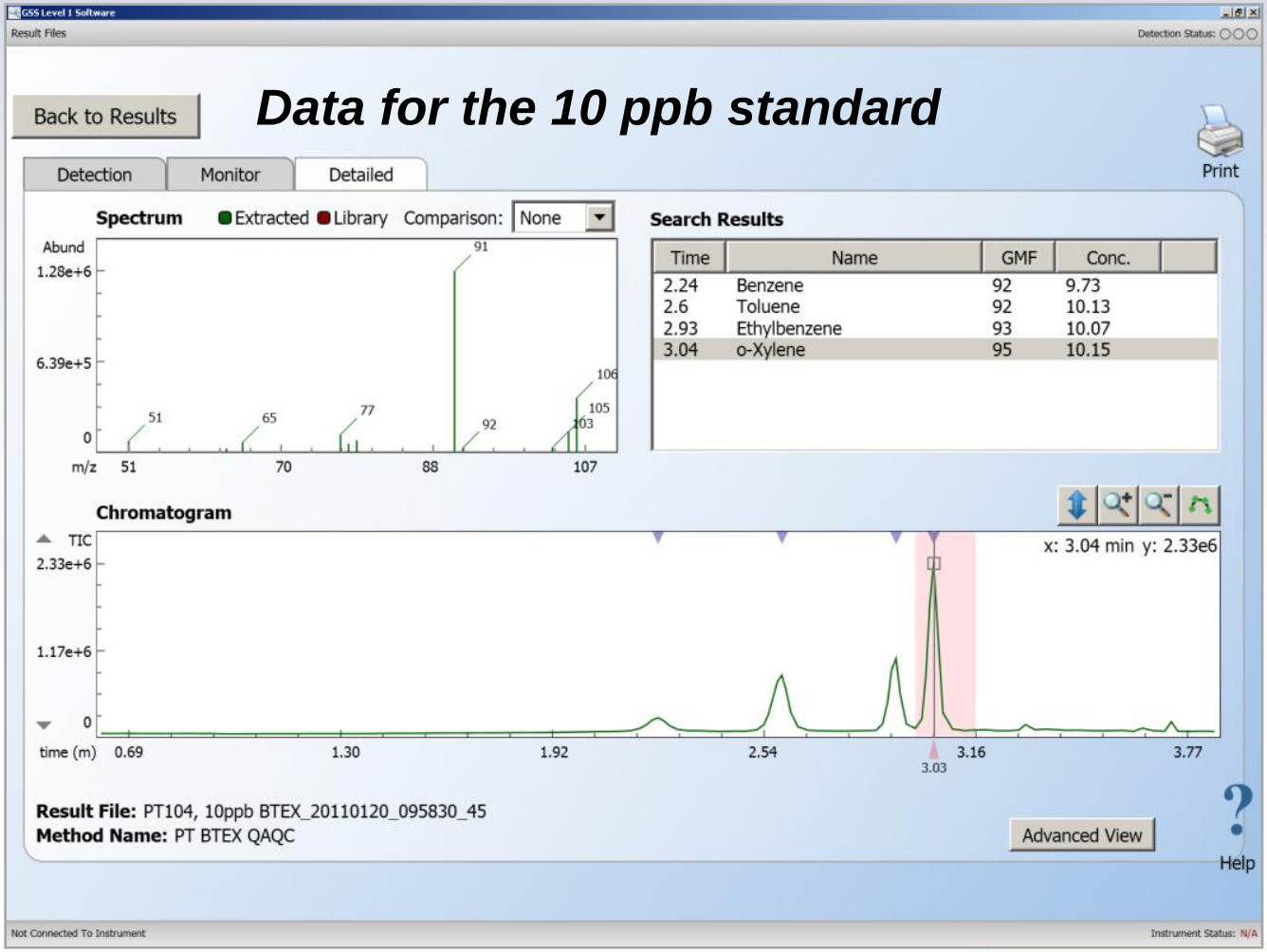
- Water Samples
- Used to purge VOCs from Water
- Docks seamlessly with Griffin 450 or Griffin 460 GC/MS
- GC/MS Preconcentrates and performs identification of VOC's in sample

Purge & Trap

Purge and Trap Applications

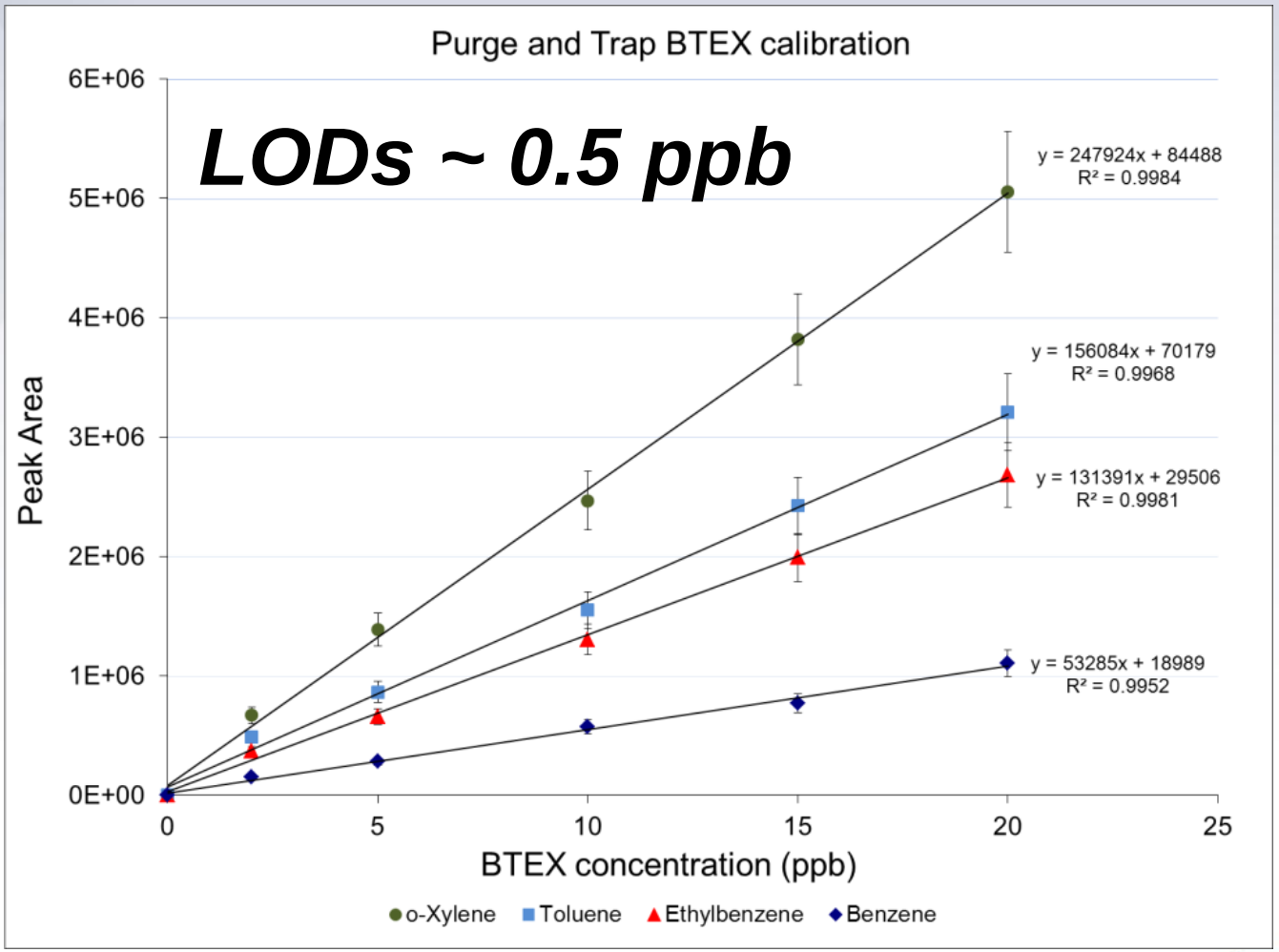
Application 1: BTEX Quantitation

- Standards prepared via dilution in distilled water
- 5 mL aliquots used for each analysis
- Purge time: 3 min; Trap temp: 45°C
- Desorb time: 2 min; Desorb temp: 200°C
- GC temp: hold 40°C 1 min, ramp to 200°C at 60°C/min
- MS Method: Full Scan m/z 50 – 425, ALC on



Purge and Trap Applications

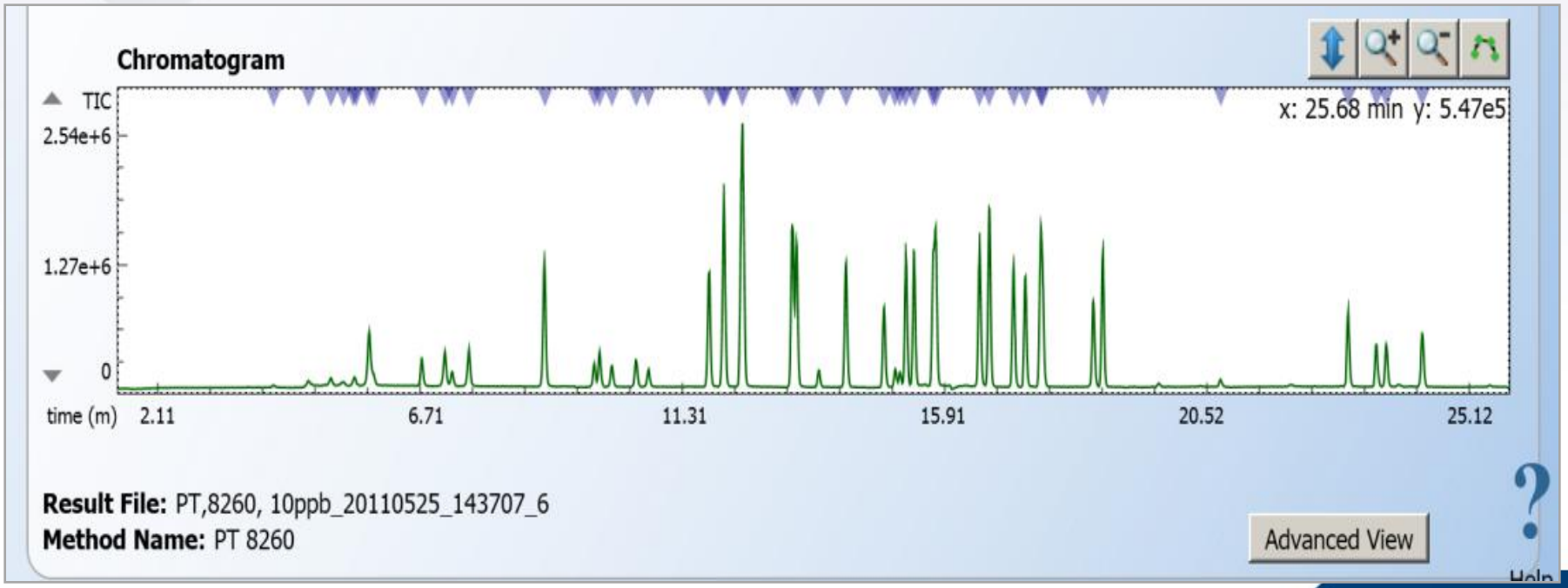
Application 1: BTEX Quantitation



Purge and Trap Applications

Application 2: VOC Mixture Analysis

- 10 ppm standard prepared via dilution in distilled water
- 5 mL aliquots used for each analysis
- Purge time: 5 min; Trap temp: 45°C
- Desorb time: 2 min; Desorb temp: 200 °C
- GC temp: hold 40°C 0.5 min, ramp to 200°C at 5°C/min
- MS method: Full Scan m/z 50 – 425, ALC on



Purge and Trap Applications

Application 2: VOC Mixture Analysis

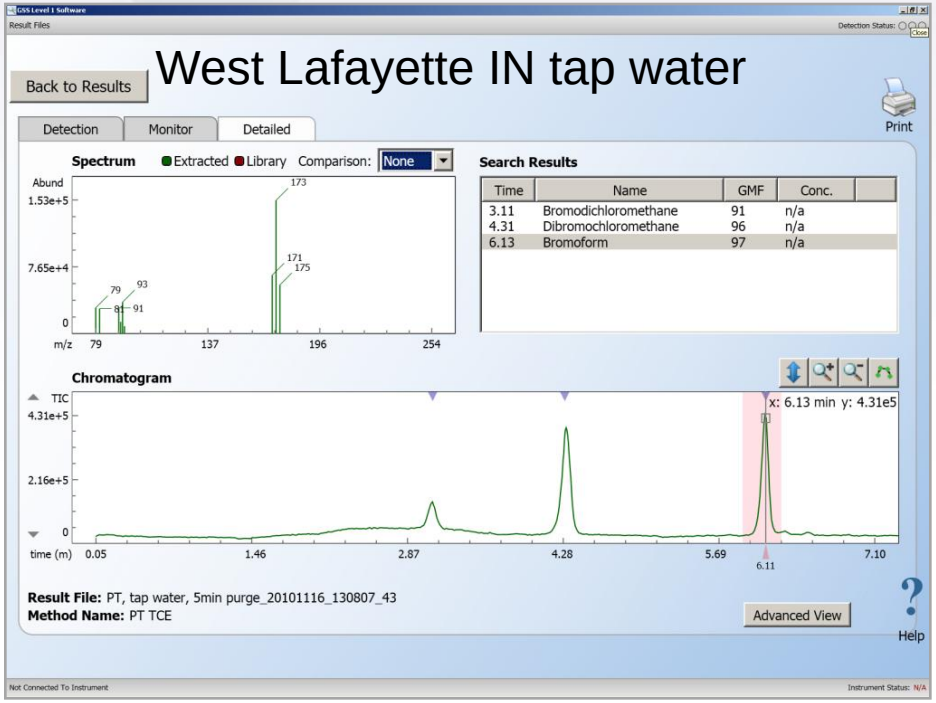
- Mixture of 52 VOCs analyzed with a 25 minute GC run on a VF-624 column (6% cyanopropyl/phenyl, 94% PDMS)
- 46 of the 52 were separated and automatically identified, with GMFs of >90 for most species
- The six undetected compounds were not trapped at the trap temperature used in this study

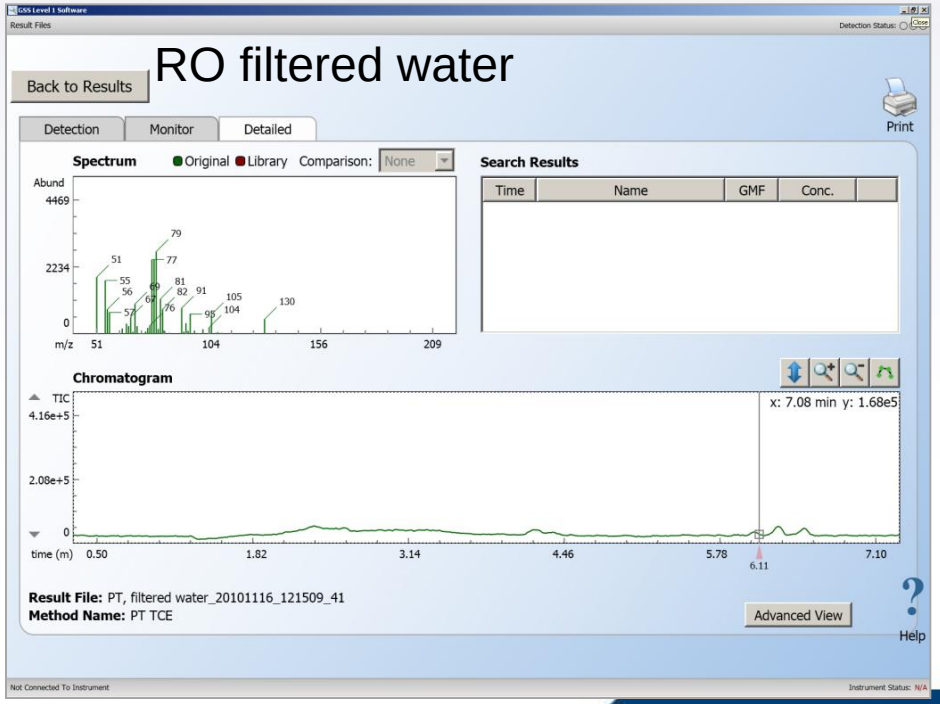
	RT (min)	Compound	GMF
1	4.15	1,1-Dichloroethane	93
2	4.76	cis-1,2-Dichloroethylene(Z)	95
3	5.16	Chloroform	91
4	5.38	1,1,1-Trichloroethane	93
5	5.55	Carbon tetrachloride	86
6	5.59	1,1-Dichloropropene	94
7	5.83	Benzene	93
8	5.9	1,2-Dichloroethane	86
9	6.76	Trichloroethylene	86
10	7.16	1,2-Dichloropropane	95
11	7.28	Dibromomethane	96
12	7.58	Methane, bromodichloro-	96
13	8.9	Toluene	91
14	9.77	1,1,2-Trichloroethane	86
15	9.87	Tetrachloroethylene	87
16	10.08	1,3-Dichloropropane	96
17	10.51	Dibromochloromethane	98
18	10.72	1,2-Dibromoethane	91
19	11.79	Chlorobenzene	97
20	12.02	1,1,1,2-Tetrachloroethane	93
21	12.05	Ethylbenzene	90
22	12.37	o-Xylene	97
23	13.24	p-Xylene	93
24	13.32	Styrene	94
25	13.7	Bromoform	94
26	14.18	Isopropylbenzene	93
27	14.85	Bromobenzene	93
28	15.05	1,1,2,2-Tetrachloroethane	88
29	15.13	1,2,3-Trichloropropane	94
30	15.23	Propylbenzene	93
32	15.71	4-Chlorotoluene	94
33	15.75	1,2,4-Trimethylbenzene	96
34	16.53	tert-butylbenzene	94
35	16.7	1,3,5-Trimethylbenzene	96
36	17.12	sec-Butylbenzene	94
37	17.33	1,3-Dichlorobenzene	92
38	17.6	p-Isopropyltoluene	92
39	17.63	1,4-Dichlorobenzene	94
40	18.51	1,2-Dichlorobenzene	91
41	18.69	Butylbenzene	95
42	20.75	1,2-Dibromo-3-chloropropane	90
43	22.99	1,2,4-Trichlorobenzene	92
44	23.48	Hexachlorobutadiene	93
45	23.65	Naphthalene	96
46	24.29	1,2,3-Trichlorobenzene	93

Purge and Trap Applications

Application 3: Disinfection By-products in Water

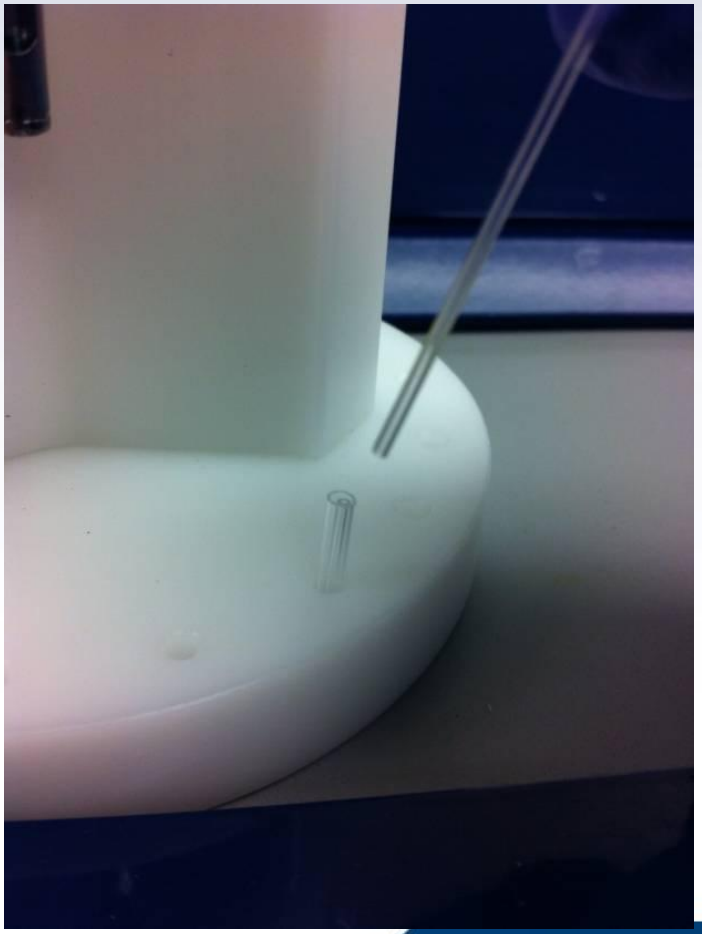
- 5 mL aliquots of tap water and water filtered with a standard reverse osmosis drinking water filter
- Purge time: 5 min; Trap temp: 45ºC
- Desorb time: 2 min; Desorb temp: 200 ºC
- GC temp: hold 40ºC 1 min, ramp to 120ºC at 5ºC/min, MS method: Full Scan m/z 50 – 425, ALC on
- LODs for the halogenated disinfection by products were in the 1 to 5 ppb range (well below the 80 ppb EPA limits)



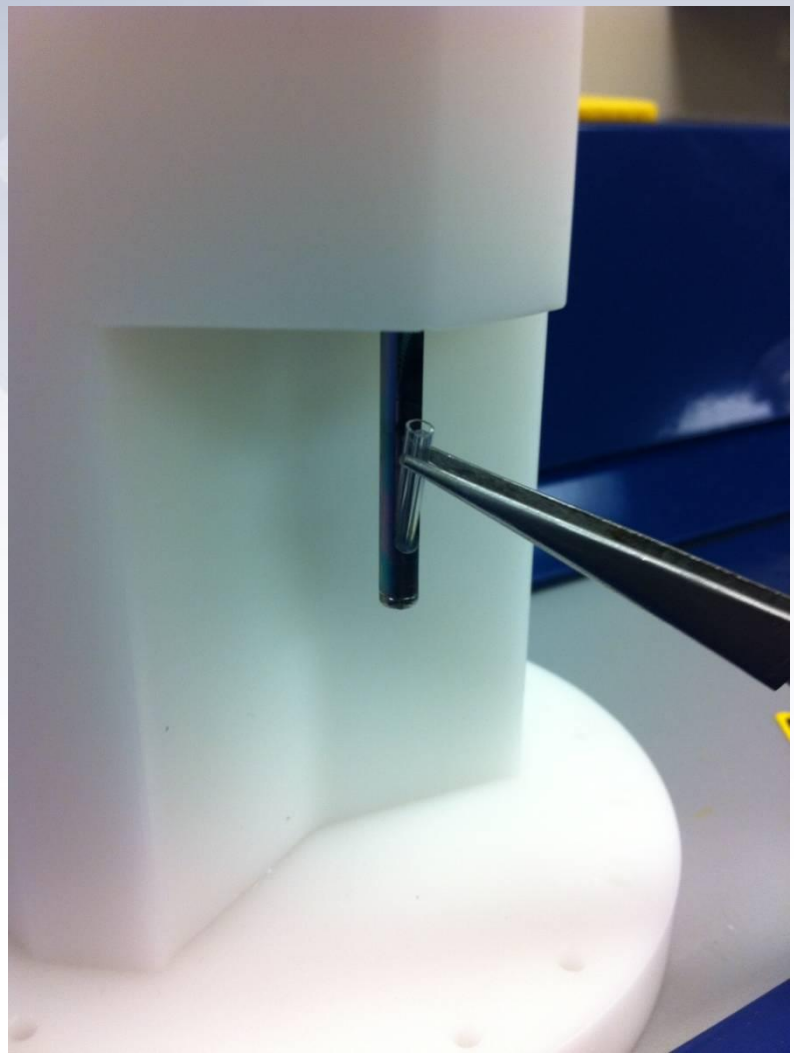


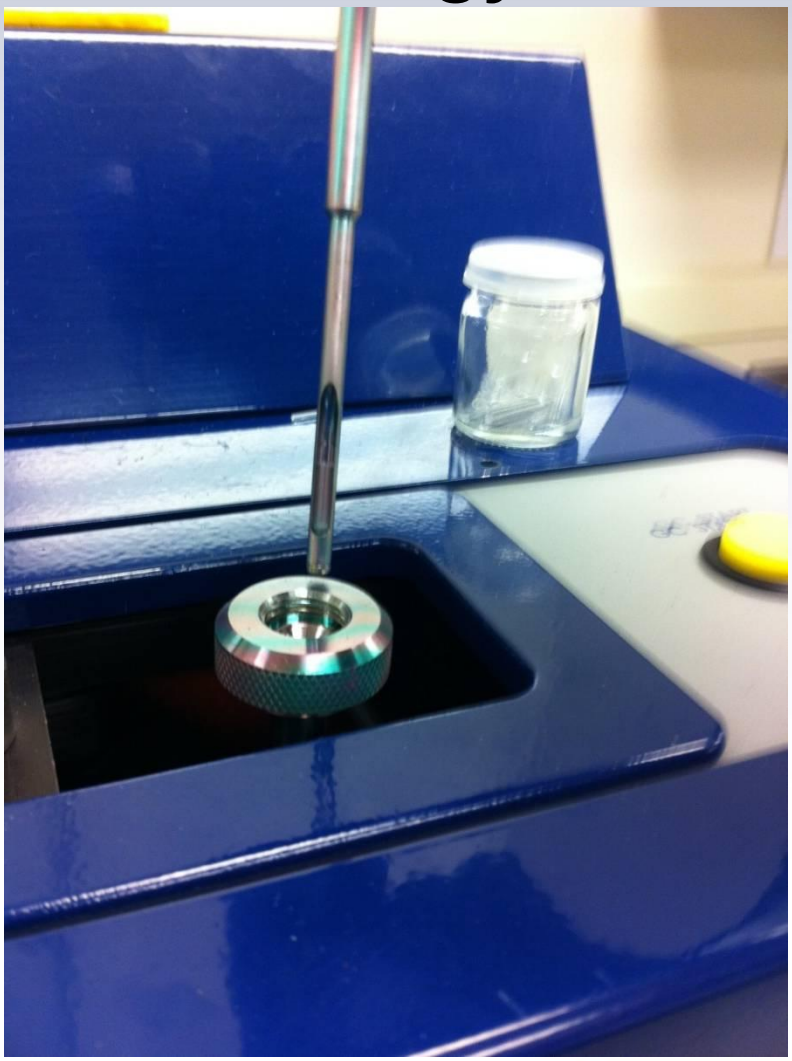
PSI Probe

Direct Sample introduction:
Where Less is More



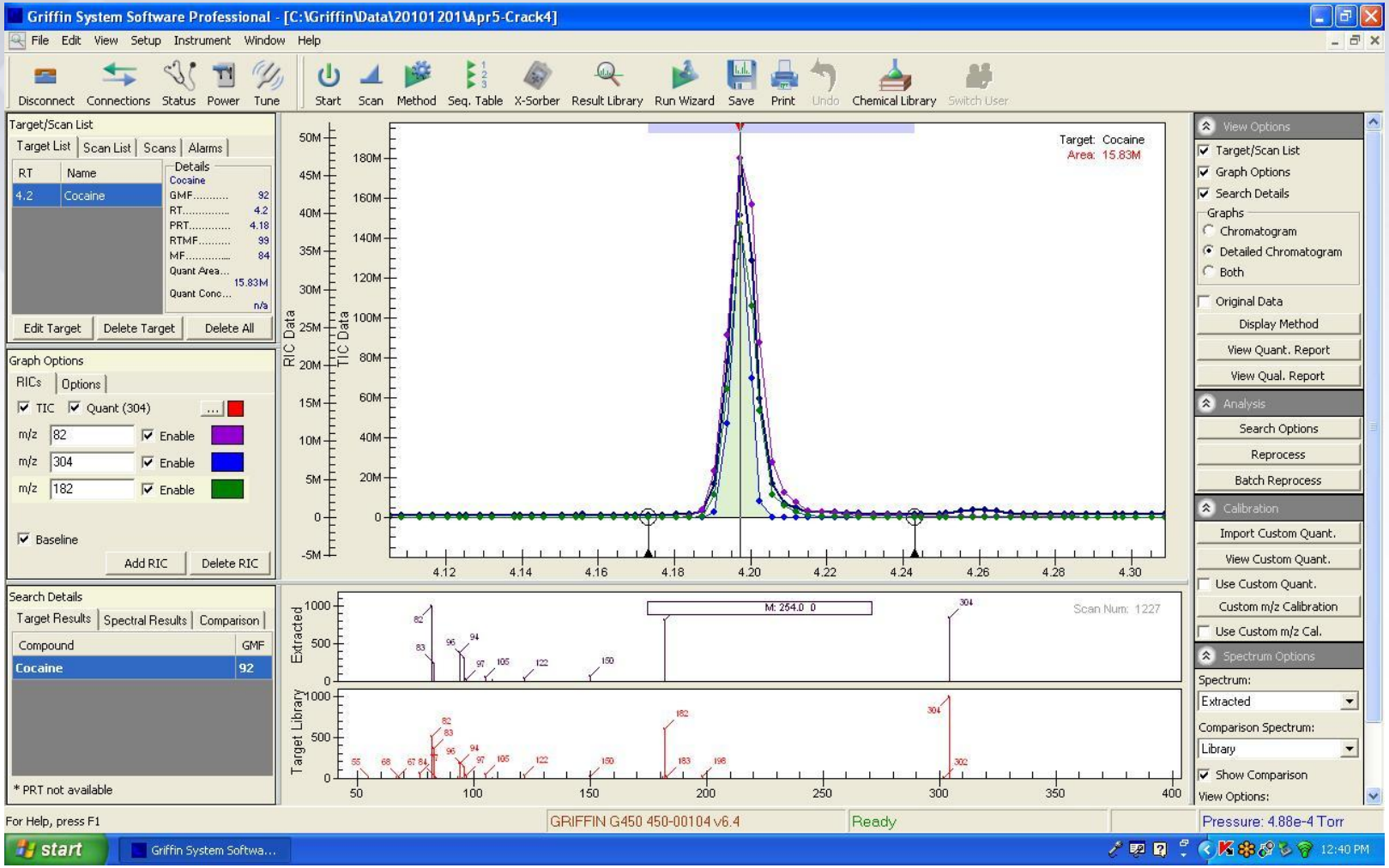
Touch-and-Go Technology



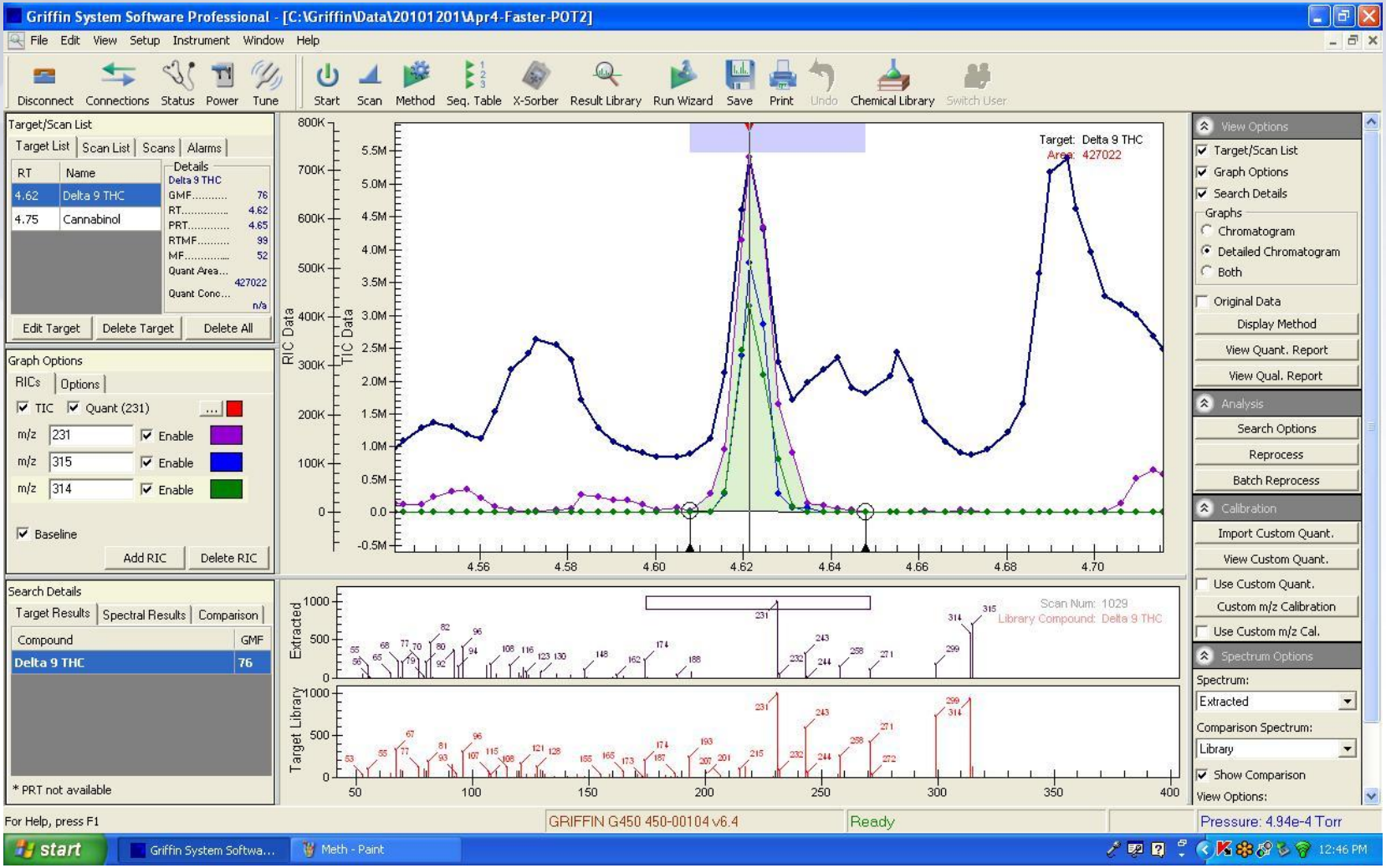


DRUG APPLICATIONS

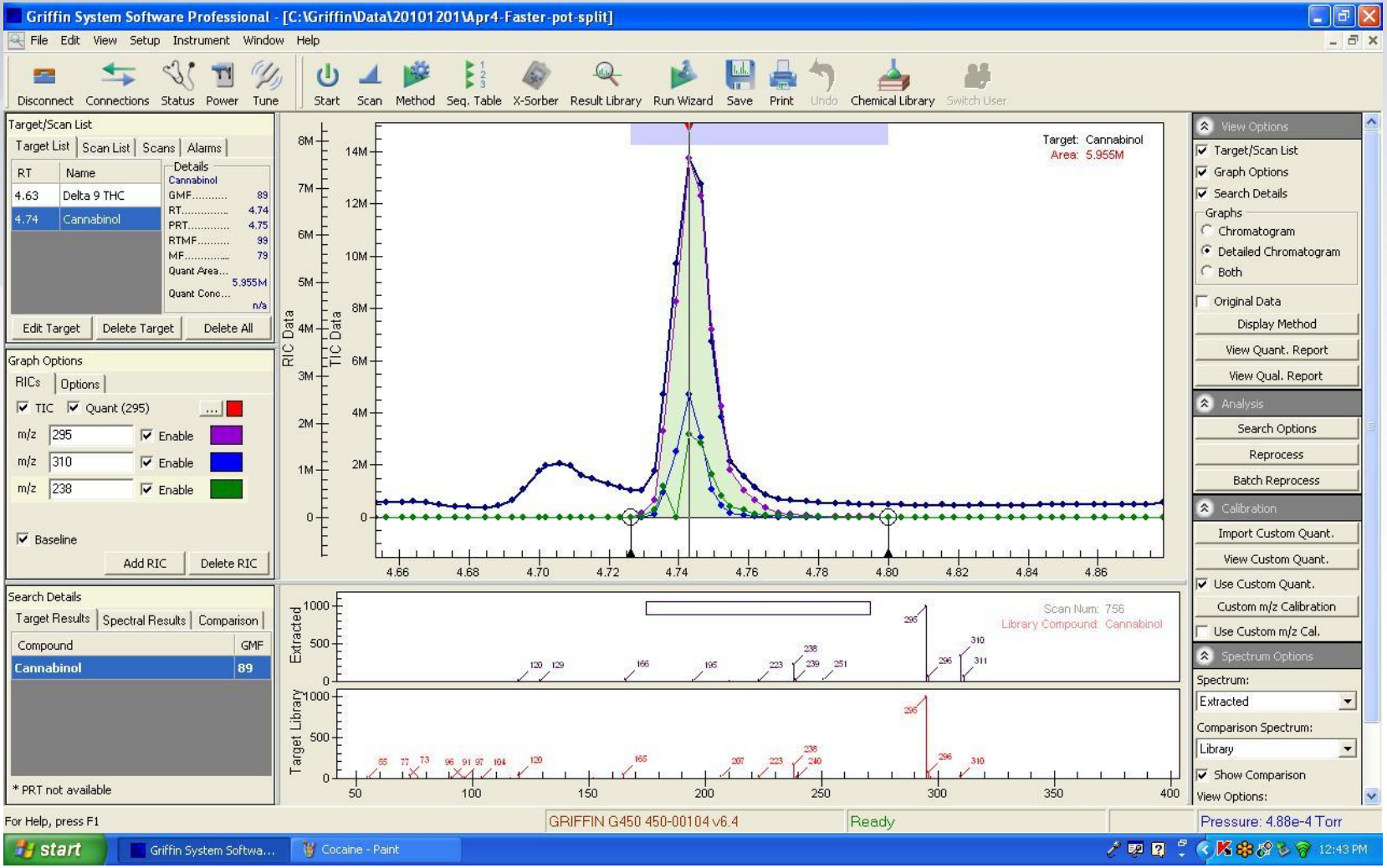
Detection of Cocaine in Street Crack



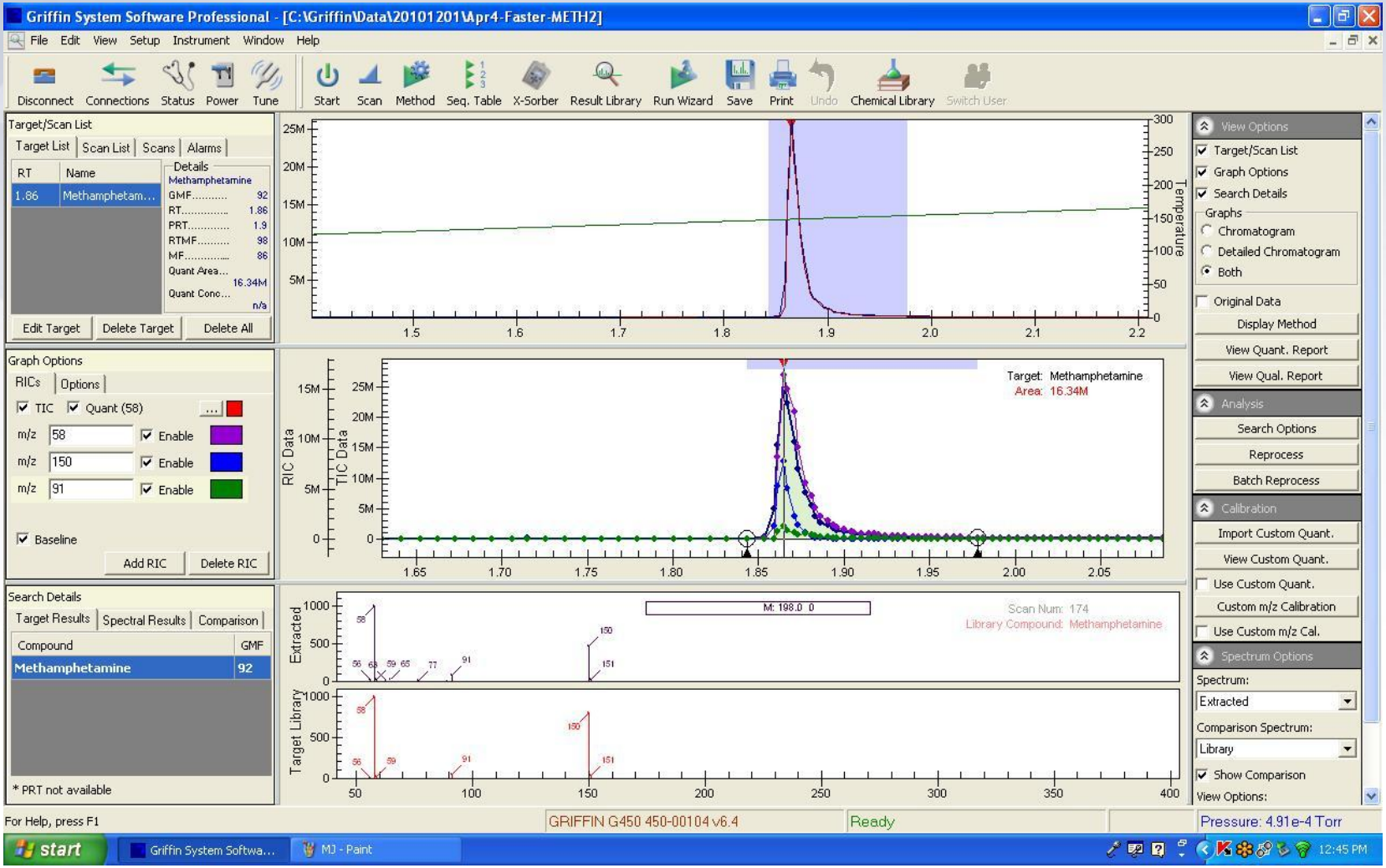
Detection of THC in Raw Cannabis



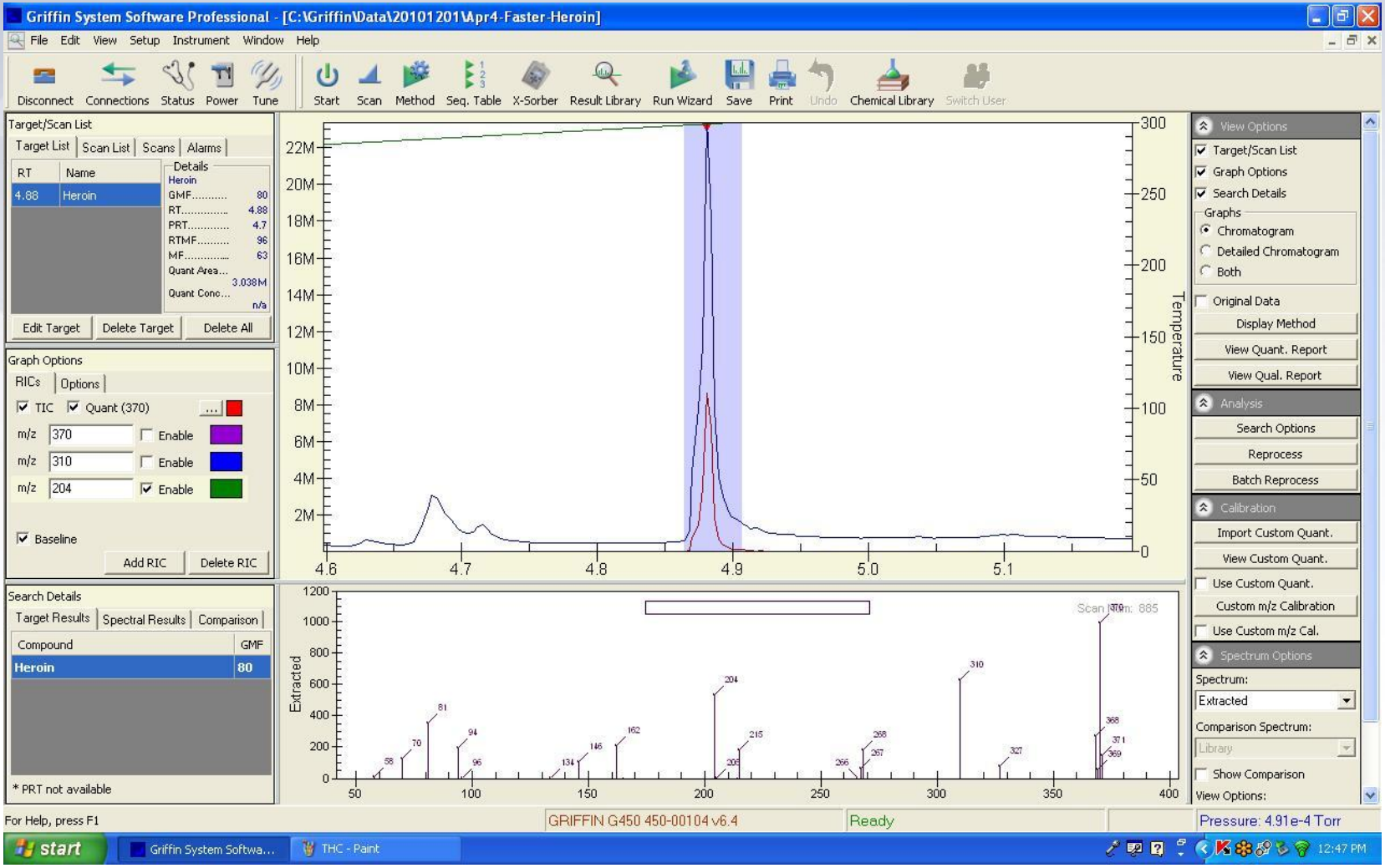
Detection of Cannabinol in Raw Cannabis



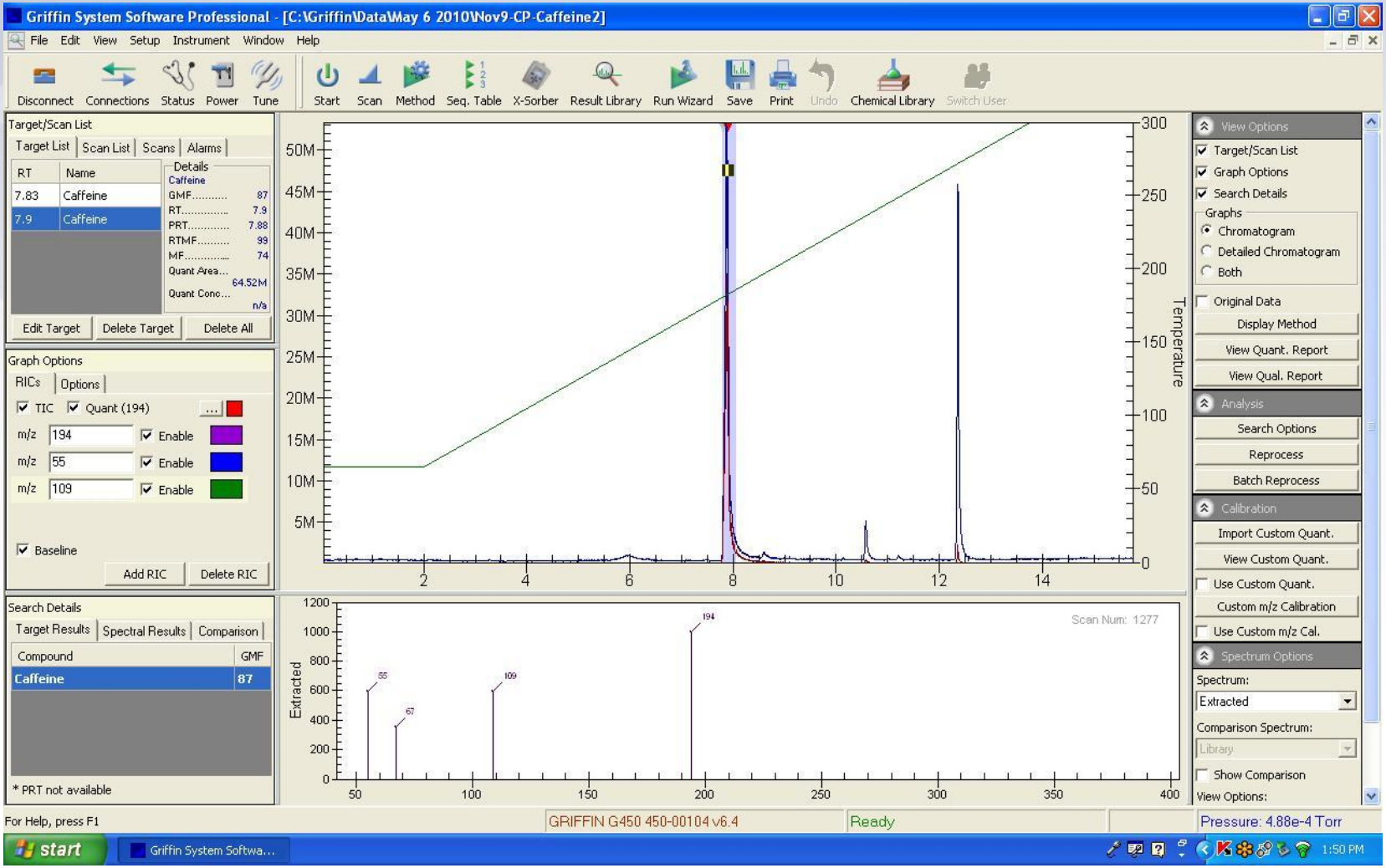
Direct Analysis of Methamphetamine



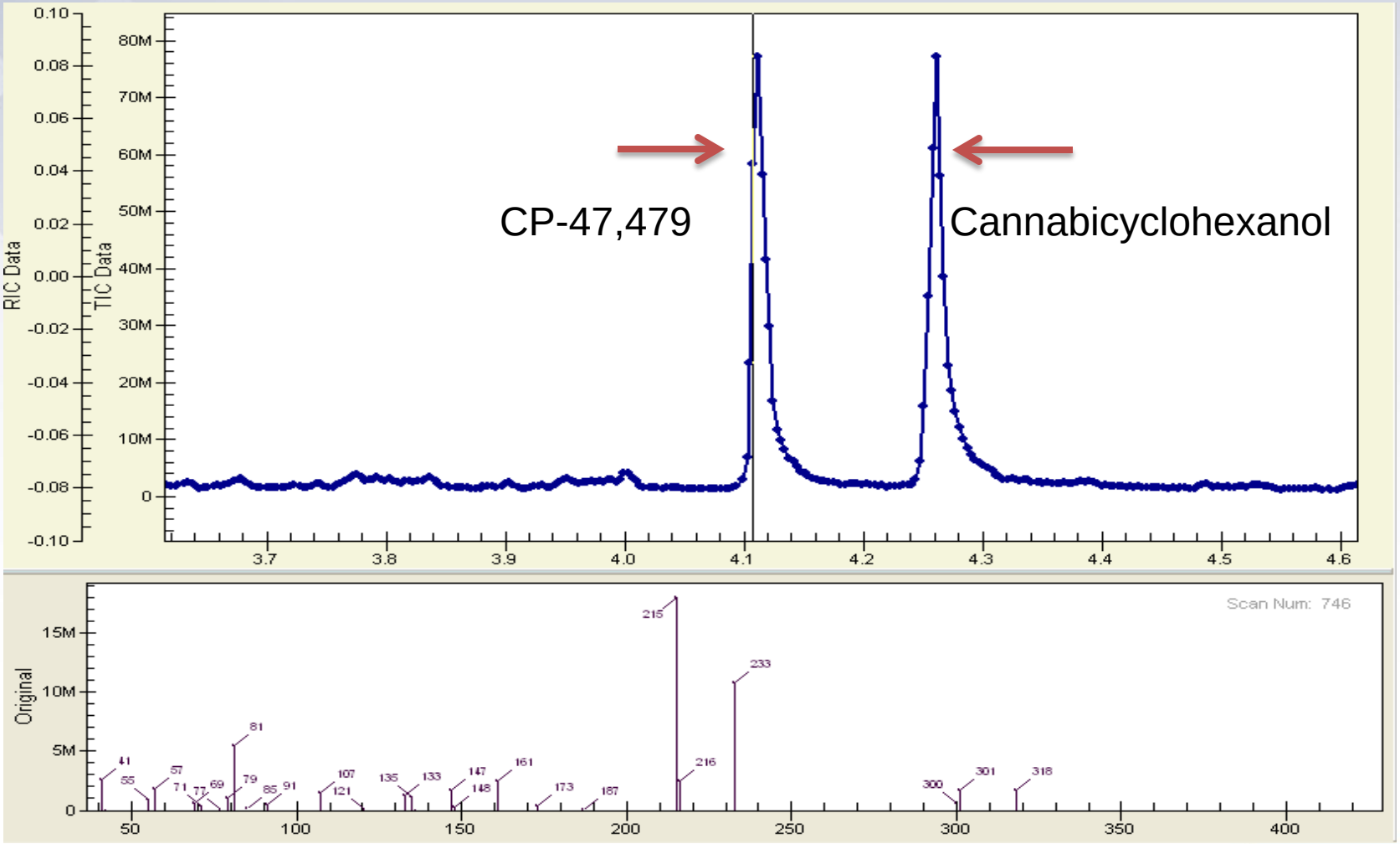
Heroin Powder - Detection



Cutting Agents – Caffeine Detection

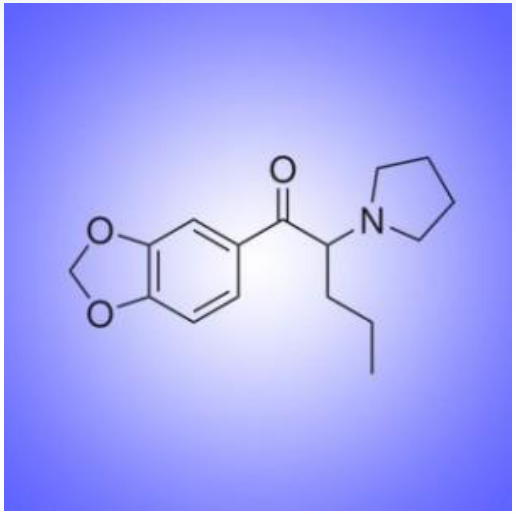


Designer Drug Analysis: Synthetic Cannabinoids – No Commercially Available Mass Spectral Libraries

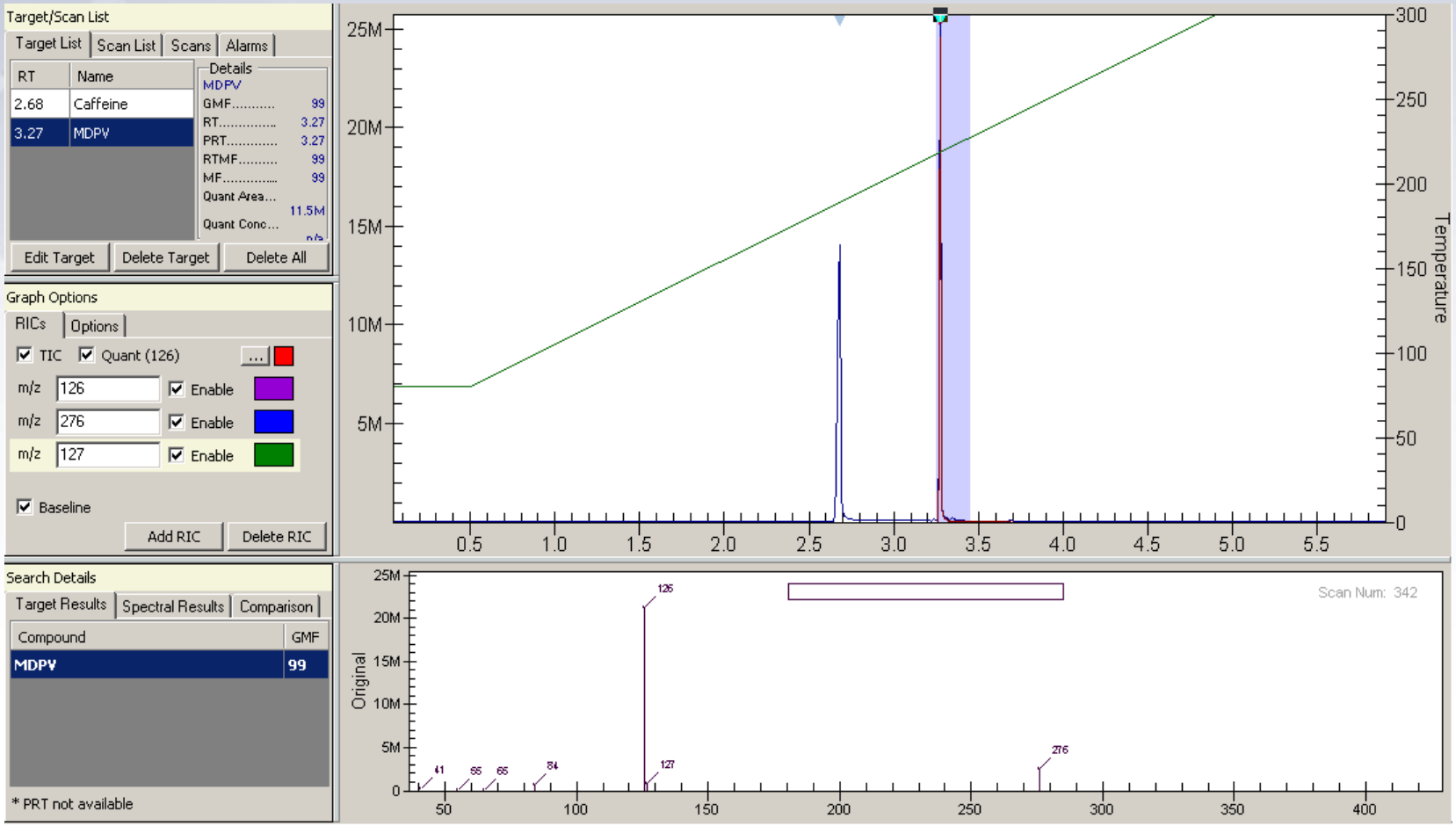


Bath Salt Analysis

- Bath salts, including those marketed under the brand names Tranquility, Ivory Wave, Vanilla Sky & Bubbles, have been outlawed in Indiana, effective July 1, 2011
- Previously could be purchased at head shops and convenience stores
- Users report effects ranging from increased libido to extreme anxiety
- Contains a chemical called 3,4-Methylenedioxypyrovalerone (MDPV) which inhibits uptake of both dopamine and norepinephrine at the post-synaptic neuronal membrane
- MDPV hit the streets in the US in 2004 as a designer drug, with stimulant effects similar to cocaine and amphetamine
- Numerous deaths in the US have been directly associated with excessive MDPV consumption

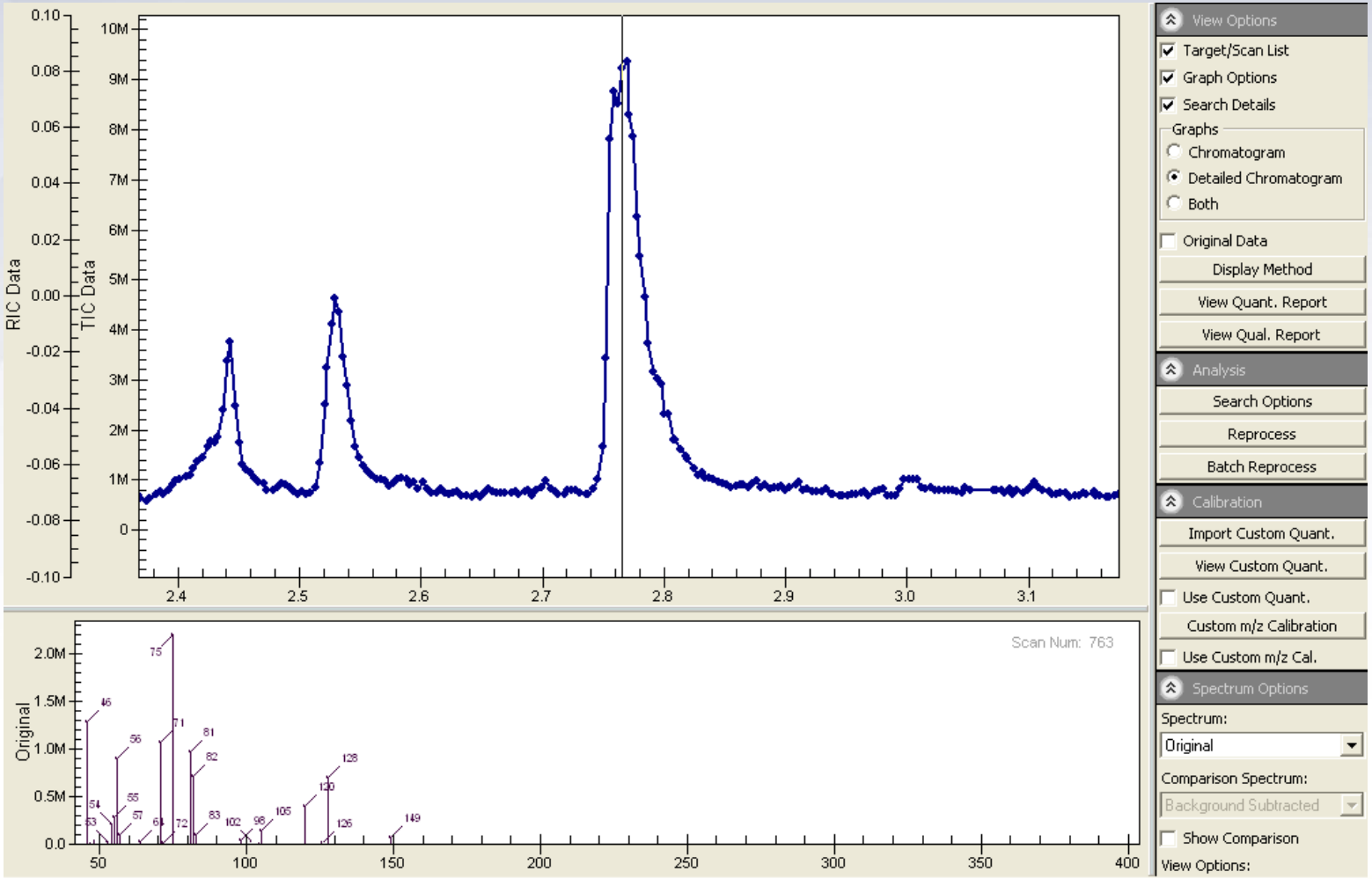


Designer Drug Analysis:
Detection of 3,4-Methylenedioxypyrovalerone (MDPV) in “Bath Salts”
(Determined To Be Cut With Caffeine)



SECURITY APPLICATIONS

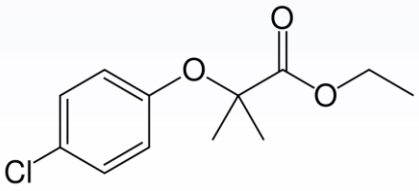
Direct Detection of RDX
Det Cord



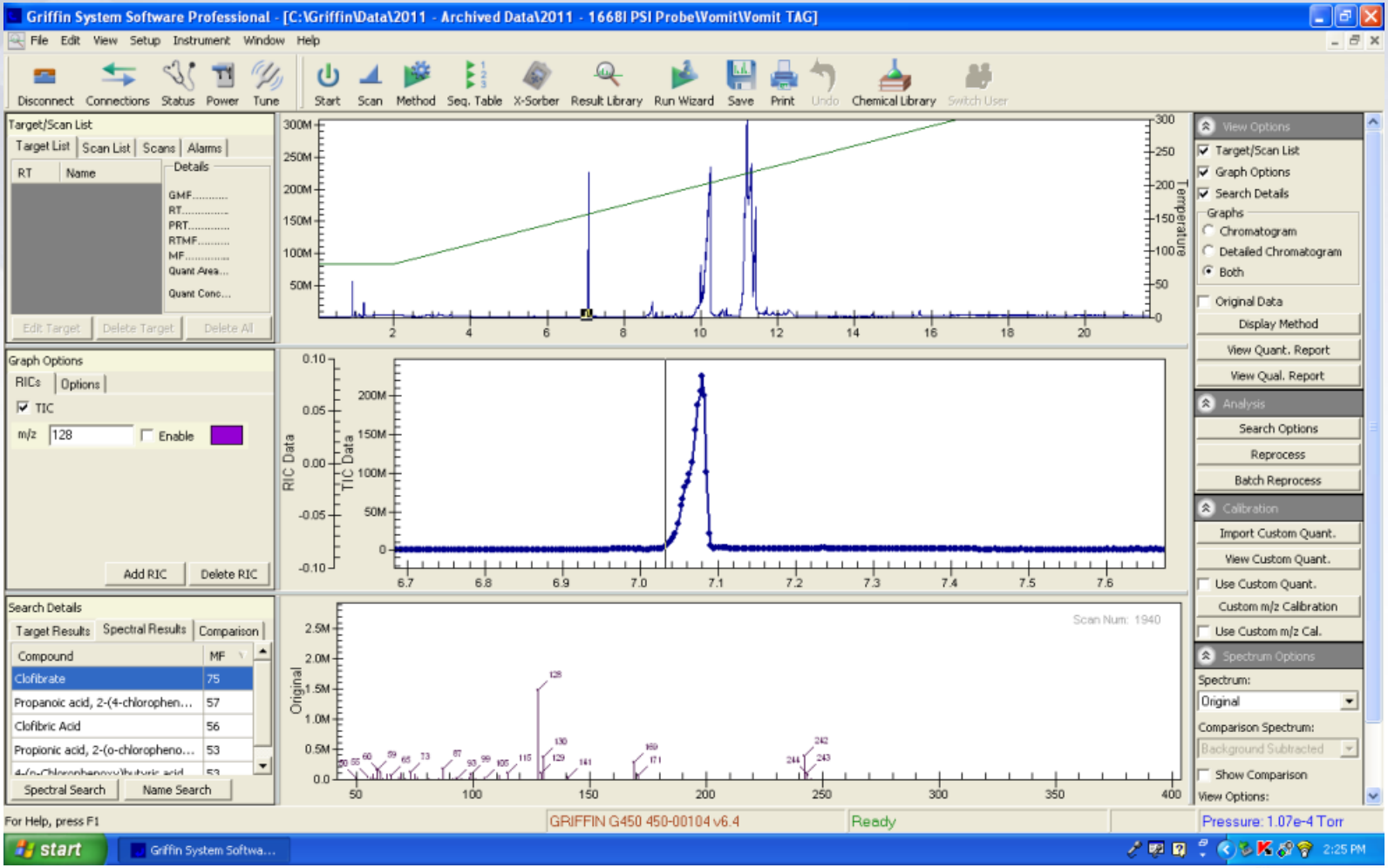
FORENSIC TOXICOLOGY APPLICATIONS

Forensic Toxicology – Analysis of Vomit

- Canine vomit sample analyzed by TAG
- Canine presented to owner with symptoms of nausea & vomiting
- Determination was made that canine got into its owner's supply of Clofibrate, a cholesterol lowering medication



Forensic Toxicology – Direct Detection of Clofibrate in Vomit



Forensic Toxicology – Analysis of Post-Mortem Stomach Contents

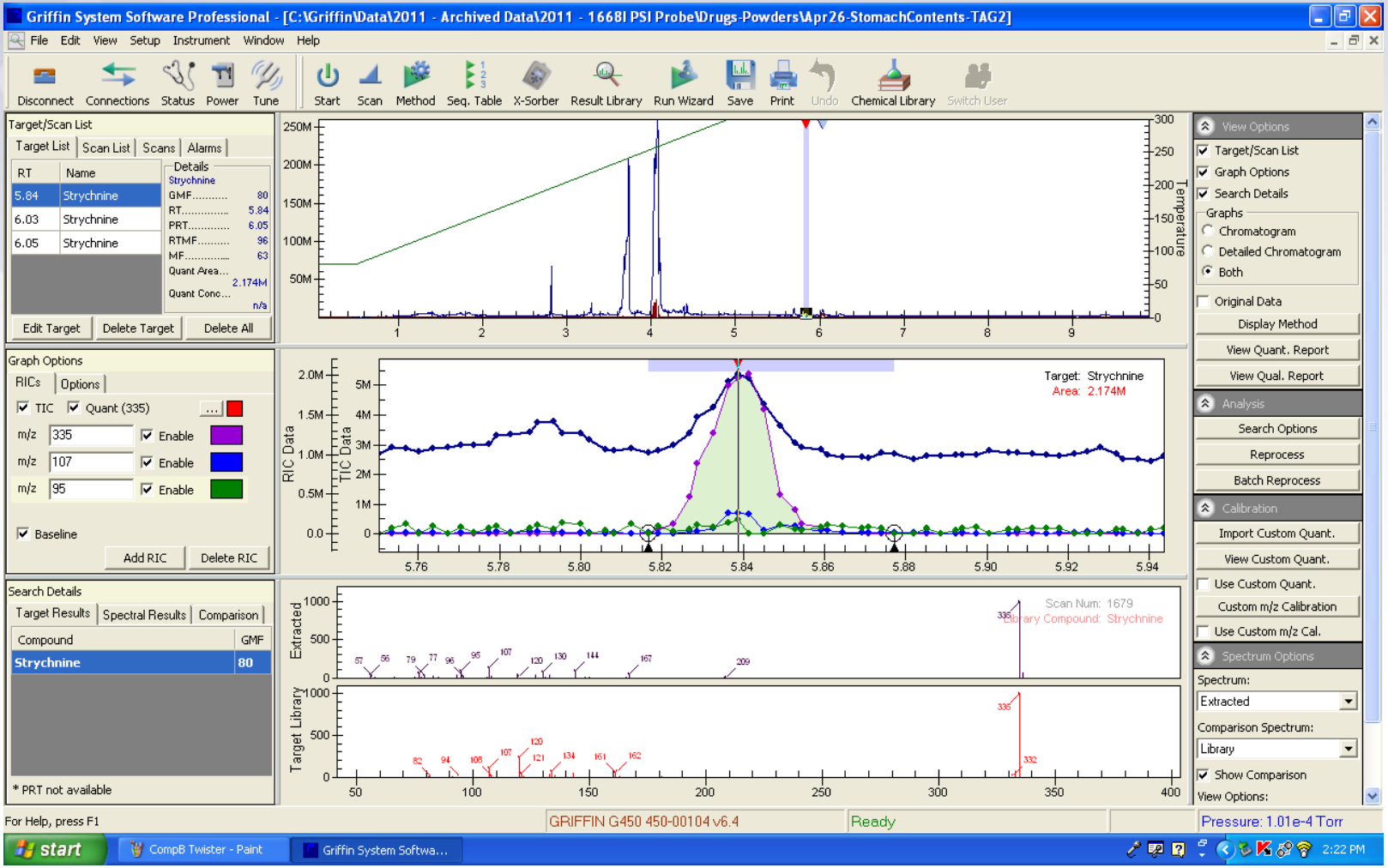
- The most common malicious poison used to kill canines in Oklahoma is Strychnine
- Strychnine is commercially available coated on Milo grain, used primarily for the control of gophers & rodents

LOOK AWAY NOW

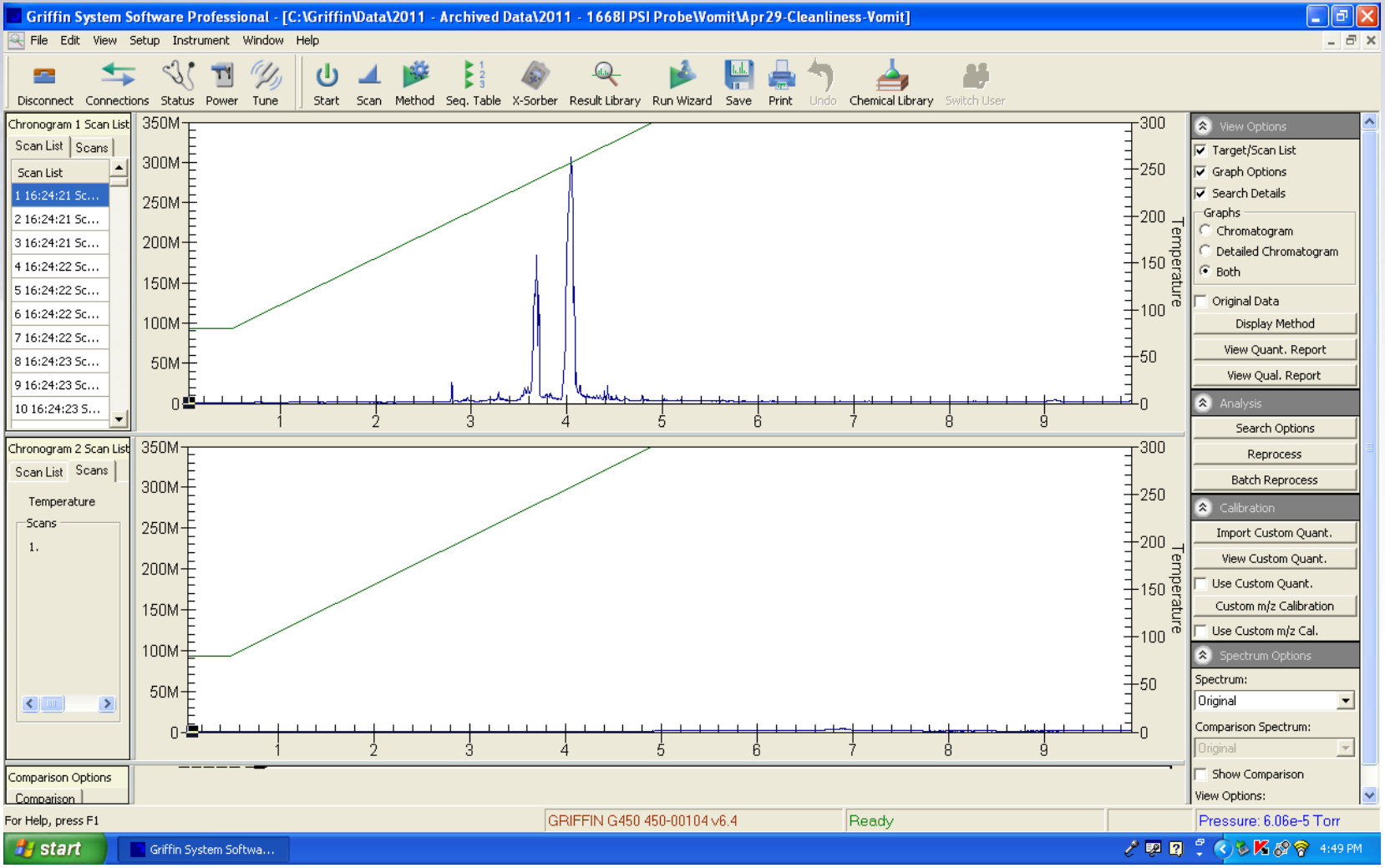
Forensic Toxicology – Strychnine Poisoning

- Strychnine is a natural alkaloid, extracted from the seeds & bark of the Strychnos Nux Vomica Tree
- Strychnine inhibits glycine, an inhibitory neurotransmitter, resulting in a violent death characterized by severe convulsions and eventual asphyxiation due to paralysis of throat muscles
- Stomach contents were analyzed by TAG PSI-Probe technology, with positive confirmation of strychnine

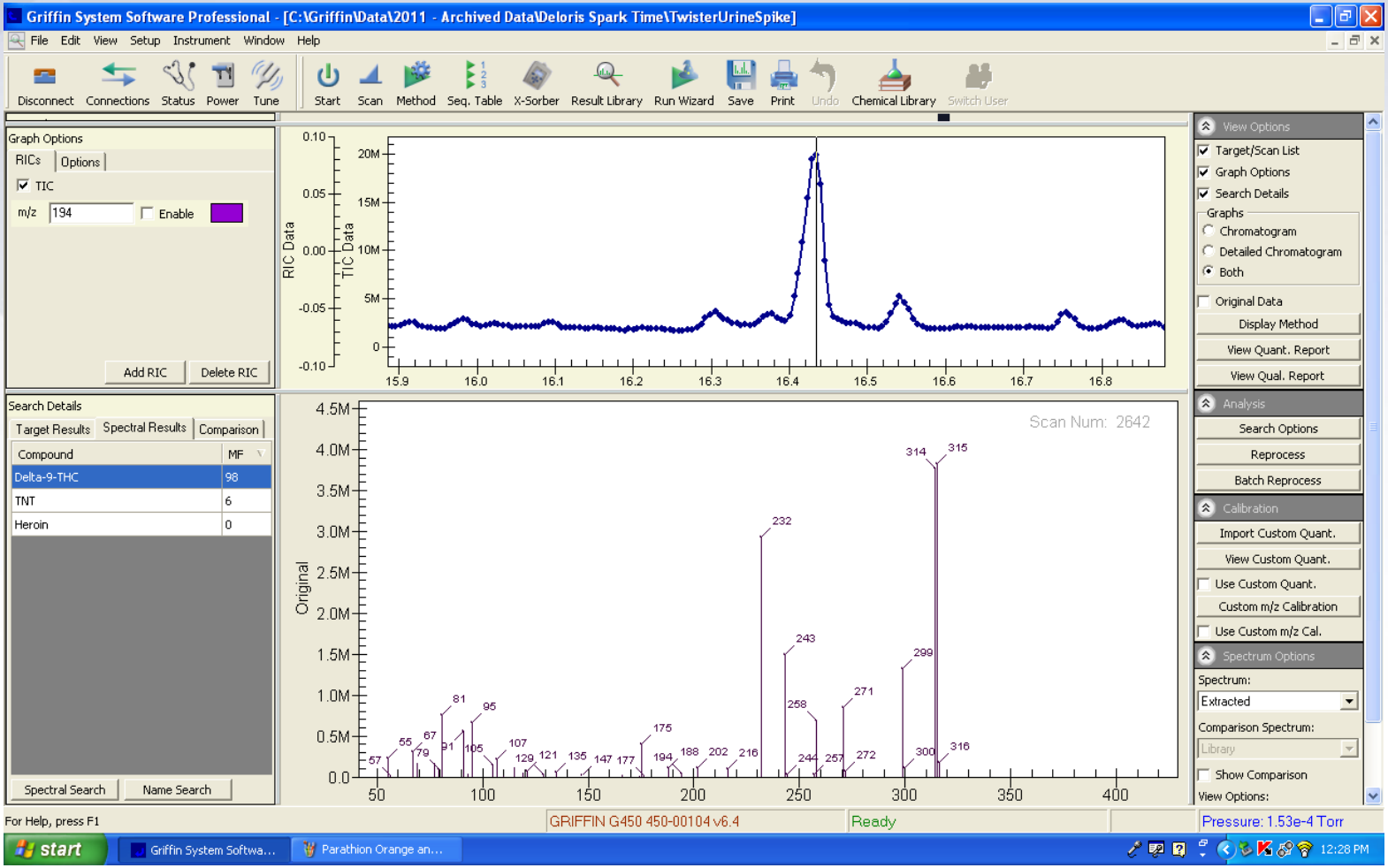
Forensic Toxicology – Direct Detection of Strychnine in Post-Mortem Stomach Contents



Chromatograms – Before & Immediately After Vomit



Twister Urine Extraction – 10mL
Griffin 450 – 50ng/mL THC in Urine
Lowest Limit Considered “Positive” For Drug Testing



Selectivity in a Complex Soup

REAL WORLD APPLICATION:

The detection of CWA's and TIC's is dependent upon the concentration of the material. When exposed to these materials, a person carries their "scent" (trace) on their cloths, skin, and other personal items. As seen with the D5 and limonene, the presence of these materials lingers for a long time, and at very tiny quantities. If a person is carrying the trace CWA on their person, the mass spectrometer can be used to detect it.