

GC-MS Analysis of VOCs in Air Using Simultaneous SIM-Full Scan

OR

What's New in TO15 Whole Air Analysis



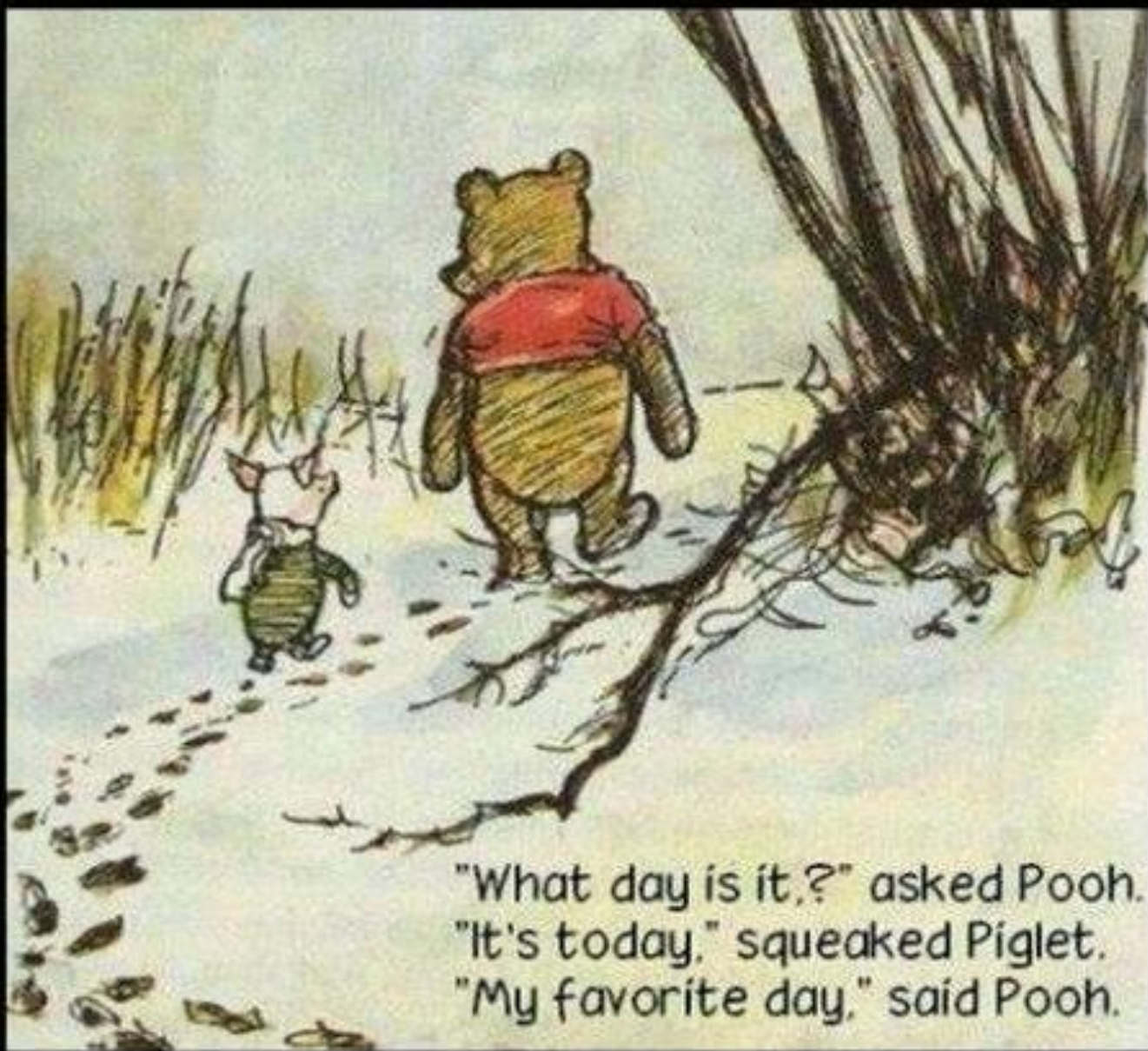
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Region 4 Air Analysts



Reason for the Subtitle

- Got bored focusing on the original topic even for 20 minutes
- Figured you would too
- Do have some interesting new instruments and methods
- Cool closing video!





"What day is it,?" asked Pooh.
"It's today," squeaked Piglet.
"My favorite day," said Pooh.

Entech 7200/7650 - Upgrade

New Features

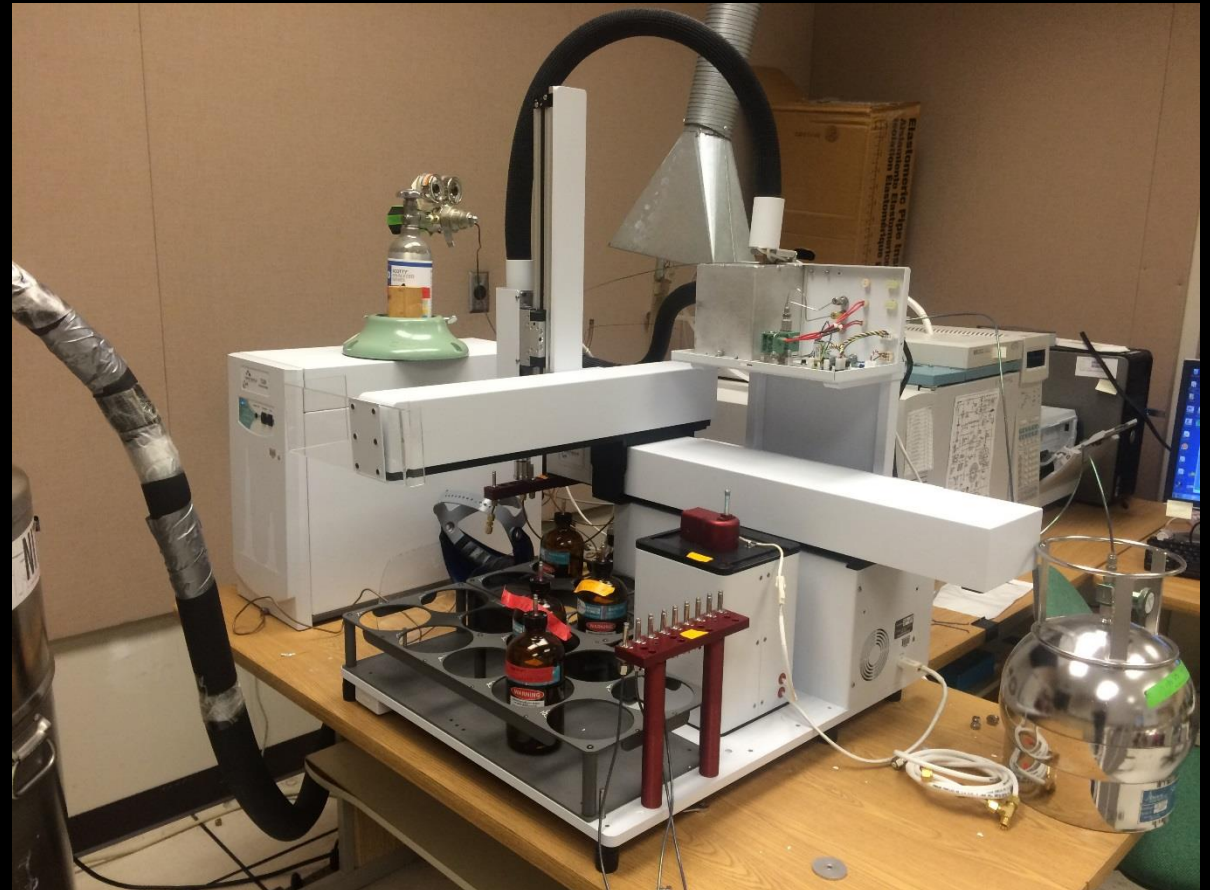
1-cc and Million air loops: 0.1-0.001 cc
high concentration samples like soil gas

Robotic arm can also sample 500-1500 cc
bottles or cans – dedicated lines to minimize
cross-contamination

Disadvantages

Can't sample cans effectively at pressures
below 13 psia

Million air loop isn't quite perfected



Markes Unity CIA

Differences from Entech
No liquid N₂ needed –
can supposedly analyze
up to 15 liters of sample

Disadvantages



Entech 4700 Precision (Static) Diluter

Differences from Entech 4600 **Dynamic** Diluter

Advantages

- Can-to-can dilutions performed automatically
- Measures pressures to .01 psia so standard preparation more precise

Disadvantages?

- No in-line humidification
- But can simulate soil gas 40% humidity – 150 uL at 30 psia



Entech 3100D Can Cleaning System

Differences from the 3100A-1 system

Advantages

- Holds twice as many cans
- Heating program is variable
- Run by a tablet

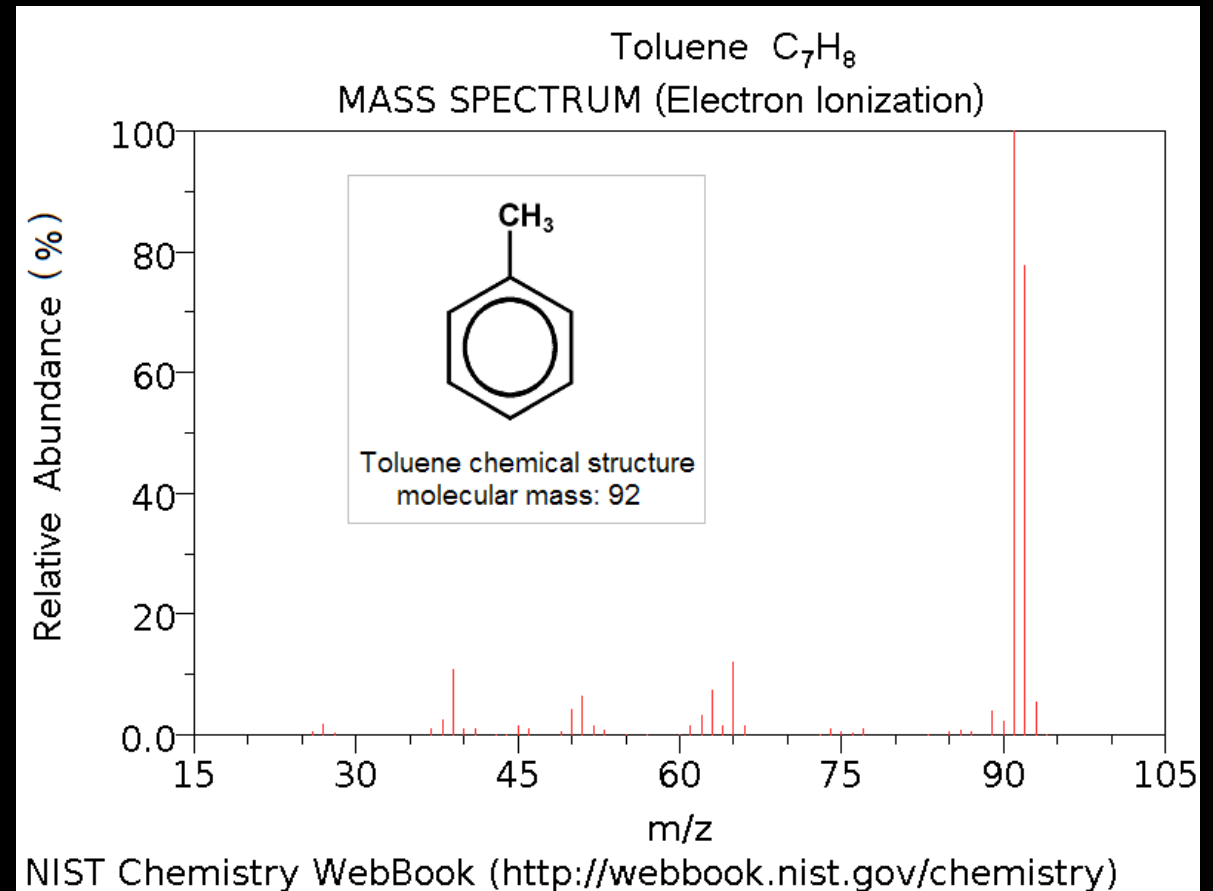
Disadvantages

- Hard to connect bottom cans
- Can't hold any cans >6 L



Synchronous SIM/Scan

- Provides library searchable full-scan spectra as well as trace level SIM data in a single analysis.
- Best applied to analyses with wide concentration ranges or in which selected components require increased sensitivity.
- Spectral quality and signal-to-noise ratios are very similar among SIM-only, Scan-only, and SIM/Scan analyses.

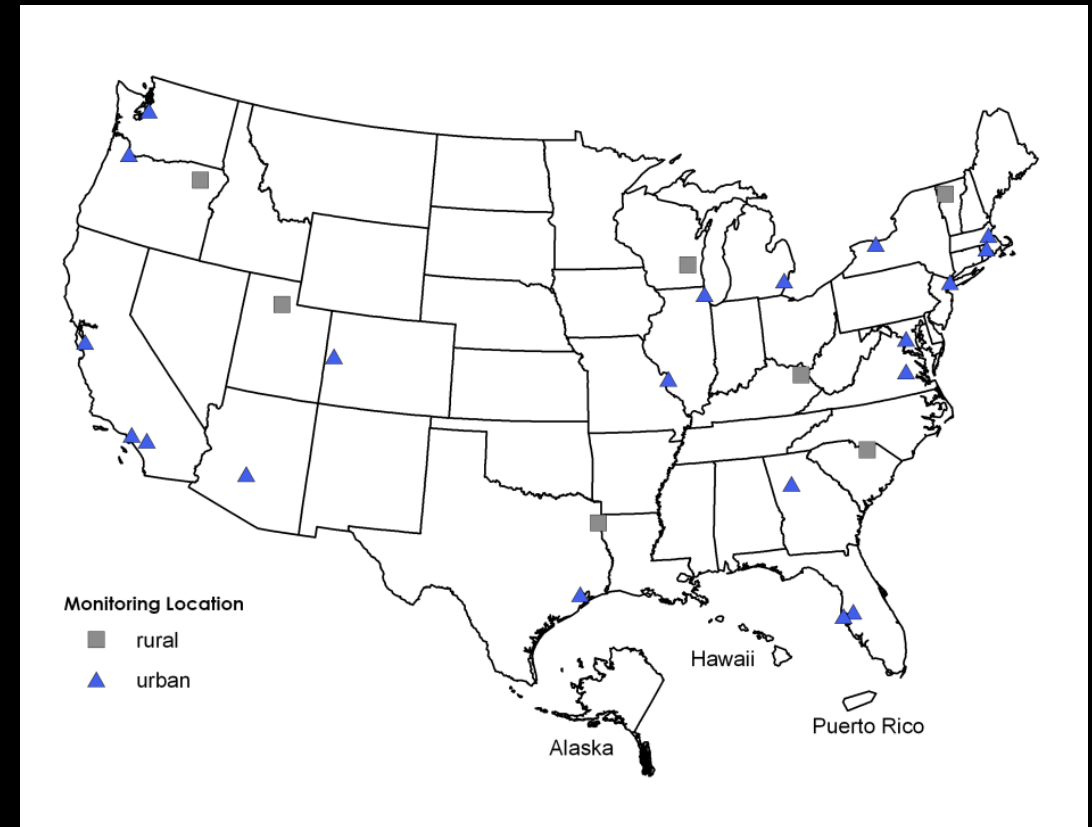


Why we are doing Synchronous SIM-Scan #1

Referee Lab for NATTS Performance Testing - PTs
(National Air Toxics Trends Stations)

Referee labs allows them to
compare against a "true
value"

Comparison of referee lab
to lab mean may show
quality issues with our
referee labs



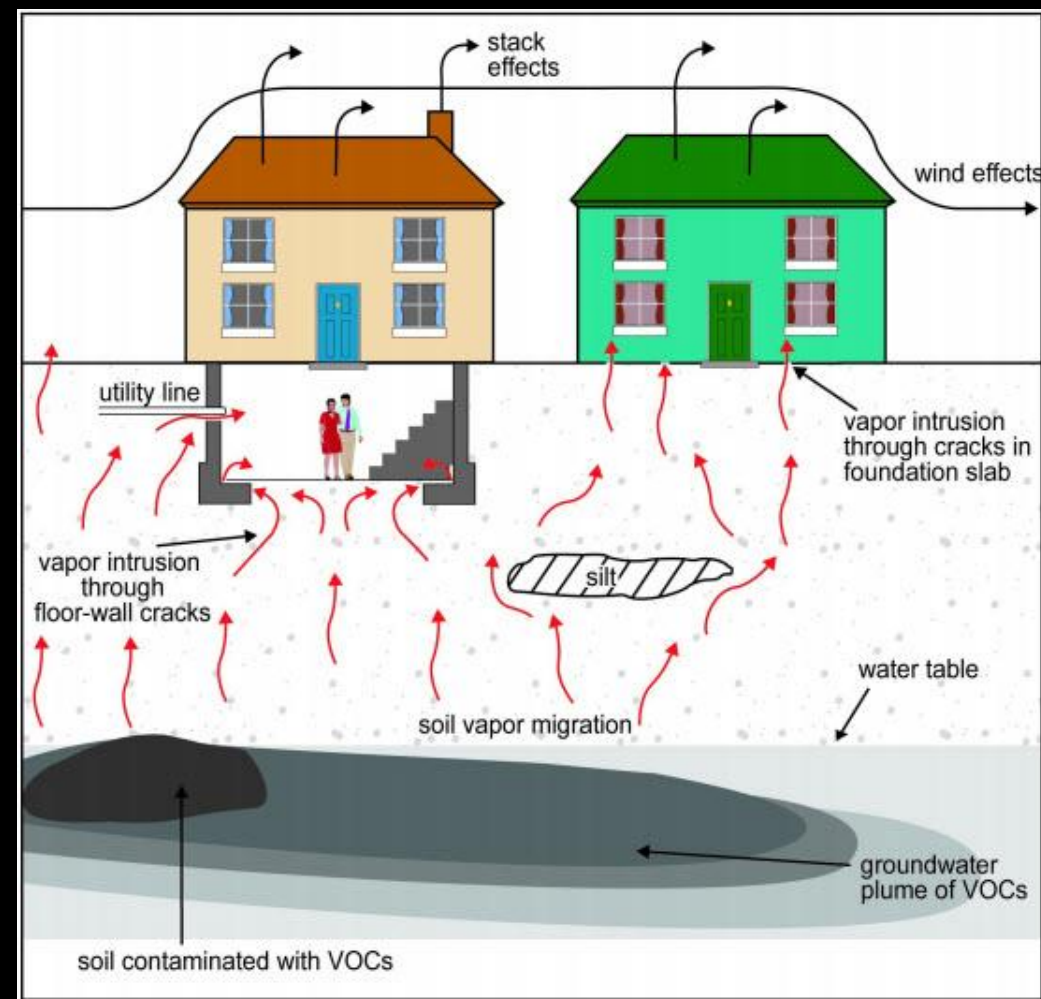
"Will continue to drop the PT spike levels to
mimic concentrations seen in ambient air." –
National NATTS QA Lead

Why we are running Synchronous SIM-Scan #2

Indoor air analysis – some of same chemicals

Vapor Intrusion - concentrations decrease, as they migrate upwards, due to diffusion and advection*, coupled with the dilution occurring when the vapors enter a building and mix with indoor air.

Advection - the transfer of heat or matter by the flow of a fluid, especially horizontally in the atmosphere, sea or ground.



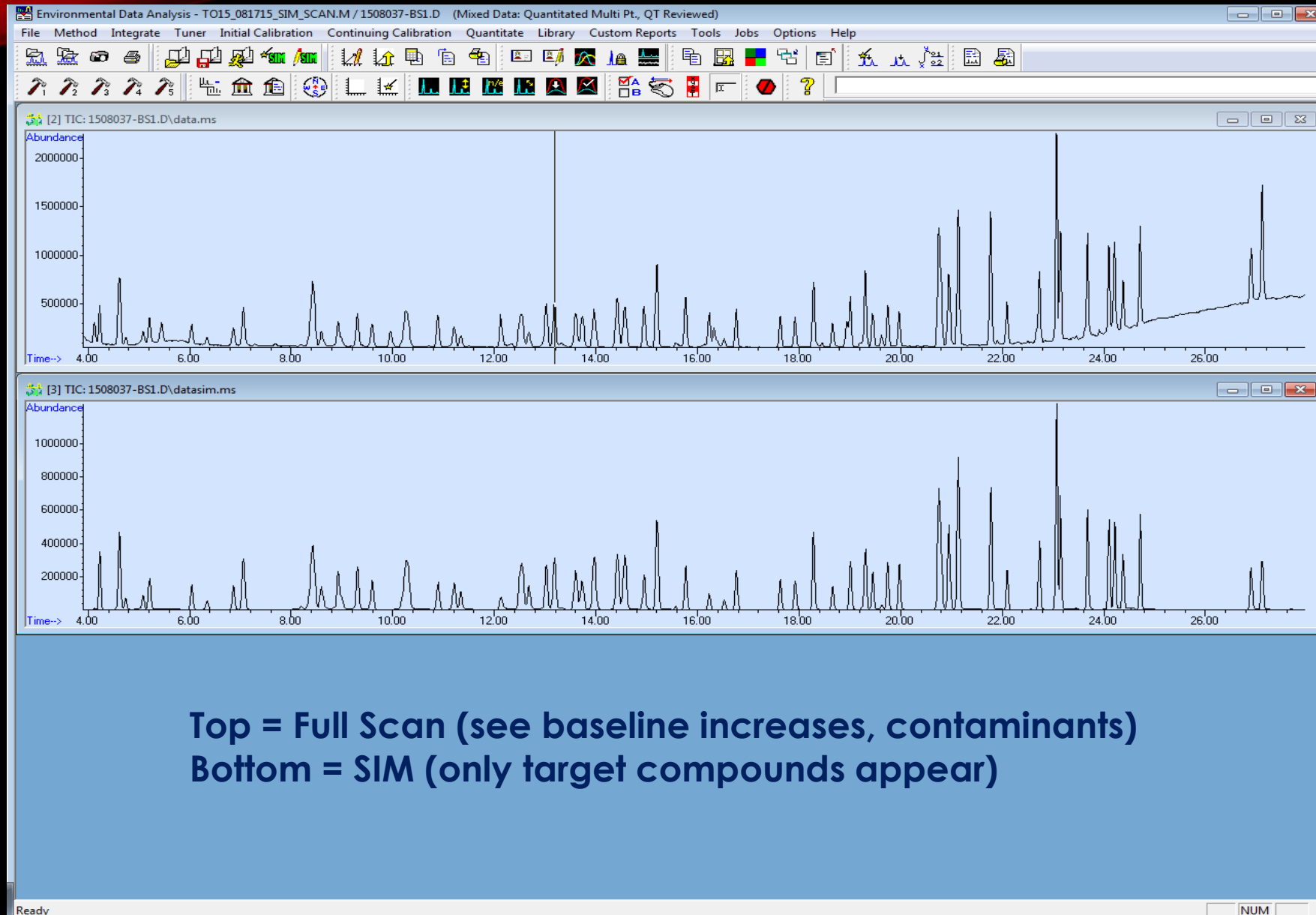
Full Scan Mode

- Monitors a range of masses known as mass to charge ratio (abbreviated m/z).
- A typical mass scan range will cover from 35-500 m/z four times per second and will detect compound fragments within that range over a set time period.
- Laboratories have extensive computer libraries containing mass spectra of many compounds to compare to the unknown analyte spectrum.
- Full Scan mode is quite useful when identifying unknown compounds in a sample and providing confirmation of results from GC using other types of detectors.

SIM MODE

- Allows for detection of specific analytes with increased sensitivity (10-100X over full scan). MS gathers data for masses of interest rather than looking for all masses over a wide range.
- Typically 2-4 ions monitored per compound and the ratios of those ions will be unique to the analyte of interest.
- To increase sensitivity, the mass scan rate and dwell times (the time spent looking at each mass) are adjusted.
- Because unwanted ions are being filtered, the signal-to-noise ratio is greatly enhanced providing an additional tool to eliminate difficult matrix interferences.

Chromatogram Comparison of Synchronous Scans



Signal-to-Noise Effects

C:\msdchem\1\data\081915\1508037-BS1.D\s_to_n.txt

Signal to Noise Report

Data Path : C:\msdchem\1\data\081915\
Data File : 1508037-BS1.D
Acq On : 19 Aug 2015 7:07 pm
Operator : CC
Sample : 1508037-BS1
Misc : _500cc Can 14677 #5081114
ALS Vial : 44 Sample Multiplier: 1

Integration File signal 1: RTEINT.P
Integration File signal 2: rteint2.p

Method : D:\msdchem\1\METHODS\T015_081715_SIM_Scan.M
Title : T015
Last Update : Wed Sep 02 16:36:51 2015

Signal Used: Mass 225; **datasim.ms**

Signal region: 27.09 to 27.15 min; height: 140736
Noise region : 26.40 to 26.60 min; Max noise 497.0, Min noise 453.0

Calculations	Value
Noise Points used	18
Average noise = (sum of noise)/points	475.3
Corrected Signal = height/Average noise	140260.7
Pk-pk noise = Max noise/Min noise	44.0
Pk-pk S/N = Corrected signal/Pk-pk noise	3187.7
RMS noise = SQRT(sum(square(noise-avg noise))/points)	15.3
RMS S/N = Corrected signal/RMS noise	9162.6

T015_081715_SIM_Scan.M Mon Oct 19 11:10:13 2015

C:\msdchem\1\data\081915\1508037-BS1.D\s_to_n.txt

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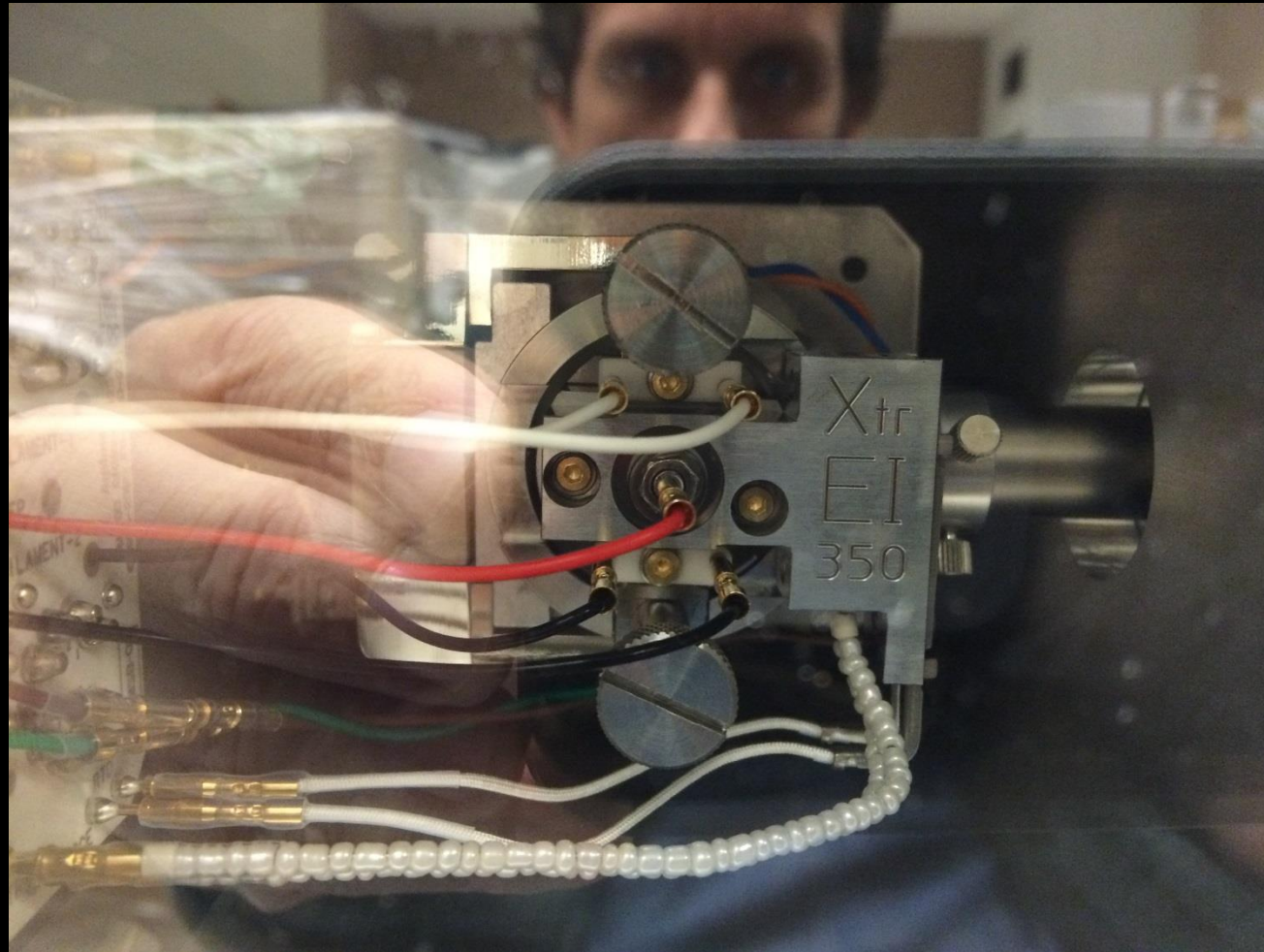
Signal Used: Mass 225; **data.ms**

Signal region: 27.06 to 27.18 min; height: 129272
Noise region : 25.50 to 26.00 min; Max noise 770.0, Min noise 241.0

Calculations	Value
Noise Points used	59
Average noise = (sum of noise)/points	481.0
Corrected Signal = height/Average noise	128791.0
Pk-pk noise = Max noise/Min noise	529.0
Pk-pk S/N = Corrected signal/Pk-pk noise	243.5
RMS noise = SQRT(sum(square(noise-avg noise))/points)	109.3
RMS S/N = Corrected signal/RMS noise	1178.0

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Setting Up AutoSIM with Existing Scan Method



Fun with Chemistry



[German dude's take on attraction](#)