



TSSPro 3.0[®]

Mass Spectrometer Data System

Developed by

Shrader Analytical and Consulting Laboratories, Inc.

General Information

TSSPro 3.0 is a complete mass spectrometer data system, designed to replace out-of-date data systems. TSSPro 3.0 provides tuning, calibration, data acquisition, and data reduction capabilities. Optional features include accurate mass determination, selected ion monitoring, target compound quantitation, library searching and linked scanning.

The data system is mouse driven and operates in the multi-tasking environment of Microsoft Windows.

Compatibility with networks and many makes and models of mass spectrometers, including magnetic sectors and

quadrupoles, provides the unique opportunity to unify multiple instruments in a laboratory with a single data system.

Please take a few minutes to see how TSSPro 3.0 can answer your mass spectrometry needs.

Special points of interest:

- PC-based mass spectrometer data system
- Stand-alone data reduction capabilities
- Compatible with a wide variety of makes and models of mass spectrometers
- Specialized projects welcome



Your LaunchPad to TSSPro 3.0

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About Shrader Laboratories

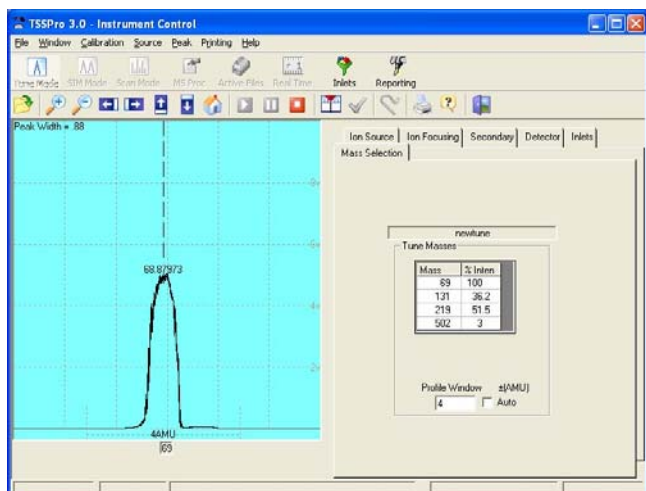
Shrader Laboratories exists to serve your Mass Spectrometry needs.

Shrader Analytical & Consulting Laboratories, Inc. was established in 1971 and moved to its present location at 3814

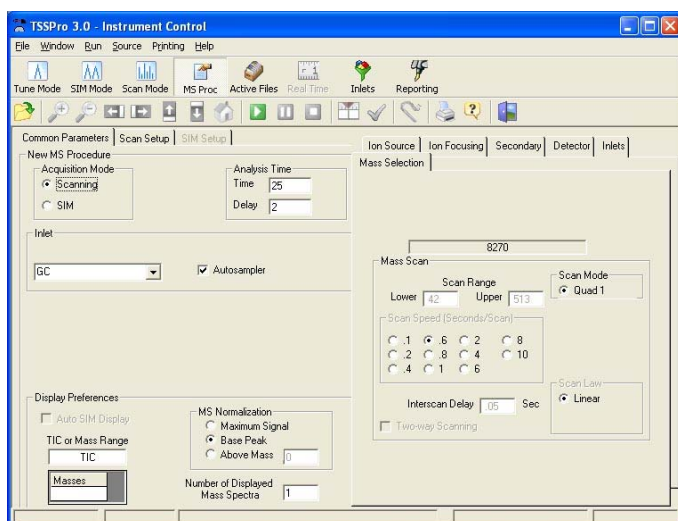
Vinewood, Detroit in 1978. It was started as a mass spectrometry service laboratory for pharmaceutical, industrial and R&D concerns.

Because of the need for a reliable mass spectrometer

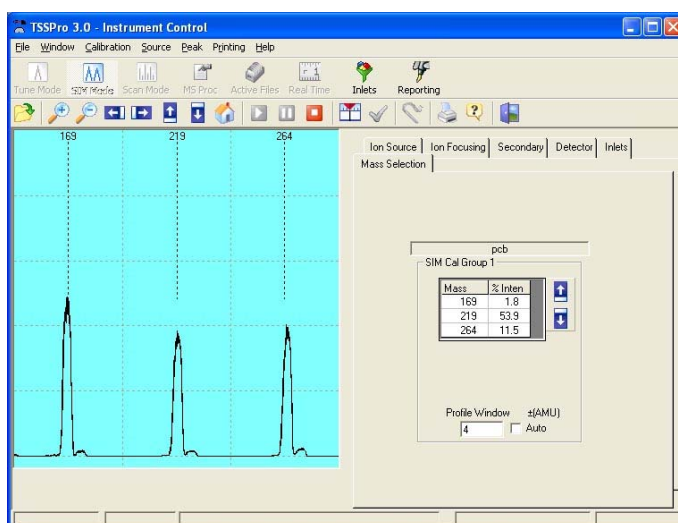
data system, The Shrader System was developed for in-house use. When the benefits of a new data system were realized, the decision was made to introduce The Shrader System to the mass spectrometry community as an



Peak display used for tuning the mass spectrometer



Define the type of mass spectra you want to acquire



SIM calibration

Tuning and Calibration

Data from a mass spectrometer is only as good as the tuning and calibration. Instrument Control displays ion profiles, single or multiple, for use when tuning the instrument. Multiple profiles can also be used for calibrating selected ion

monitoring. Mass spectra from scanning functions, magnet, high voltage, quadrupole, are displayed to calibrate the scan. Automatic and manual drag-drop methods make calibration a breeze.

Data Acquisition

How do you want to acquire your mass spectra?

accurate mass calibrations. Control GCs and autosamplers. It is all up to you as to what information you need from your mass spectrometer.

Answers to this question lie within the MS Procedure. With an almost unlimited number of ways to acquire data, the choice is yours. Scan the magnet, high voltage, quadrupoles, or combine these for linked scans, or jump into selected ion monitoring. Define multiple analyses with an autosampler or perform a single analysis. Save the mass spectra as profile, accumulated or every scan, or mass converted with your choice of centroiding methods. Indicate the presence of internal reference for

All analysis parameters are stored in procedures to ease process of acquiring data.

View real-time displays of chromatograms and mass spectra, including chromatogram ranges and auxiliary measurements.

Batch analyses can be used with Automated Data Reduction to generate unattended reports for routine analyses.

Data Acquisition Options

Selected Ion Monitoring

SIM provides increased sensitivity and allows 30 ions in 30 groups for monitoring. When performing SIM, you can jump the magnet, high voltage or the quadrupoles. For high resolution, use a lock mass for more accurate mass assignments. Fast and easy calibration is performed in Instrument Control.

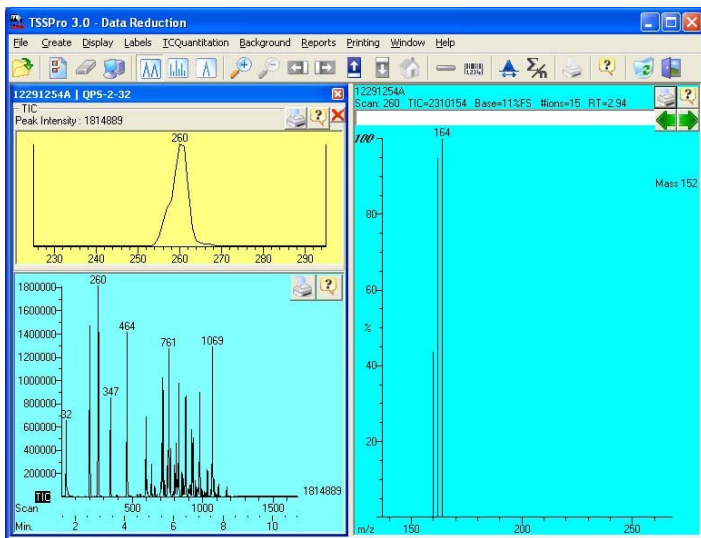
voltage outputs to link fields in the mass spectrometer to generate linked scans. Generate Product, Precursor or Neutral Loss mass spectra with the click of the mouse.

Accurate Mass

Specify the presence of internal reference to calculate accurate masses. Calibration routines in Data Reduction will assign accurate masses to the internal reference ions and recalibrate the sample ions to give accurate masses.

Linked Scanning

Utilize the multiple reference



Data Reduction display with a mass spectrum

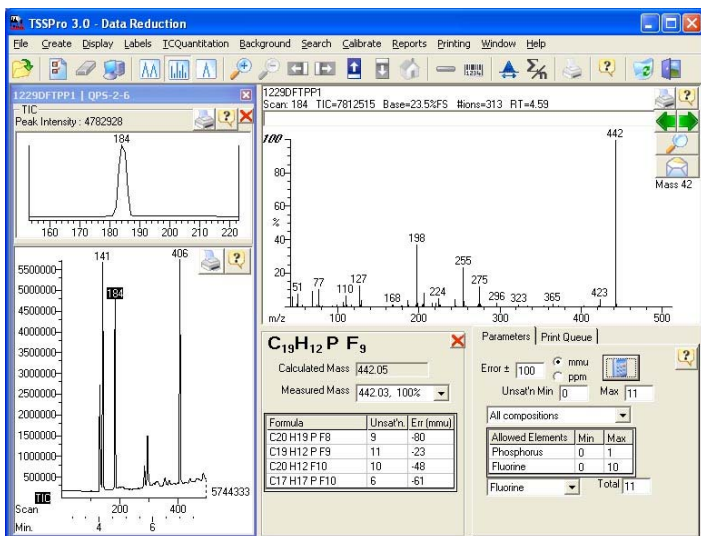
Data Reduction

How do you want to view your acquired mass spectra?

The possibilities are limitless with the high powered Data Reduction system. For starters, display TICs and chromatograms in a variety of display settings. Next, you can display your mass spectra in many formats, including bar, profile, and tabular. The choice is yours. Average them, subtract them, or create chromatograms by dragging the masses. Mass

print device, that includes printers, the Windows Clipboard, and files. User defined options specify exactly how the data will be printed.

The entire data reduction system can be used as a stand-alone program. Use it in your office for reviewing data from TSSPro 3.0 or for reviewing data from other data systems. Contact your representative for a list of formats that can be read by data reduction.



Determining elemental compositions from accurate mass data

chromatograms can be generated from a single mass or mass ranges. Integration of the peaks in these chromatograms is a simple mouse click away.

All features can be sent to the

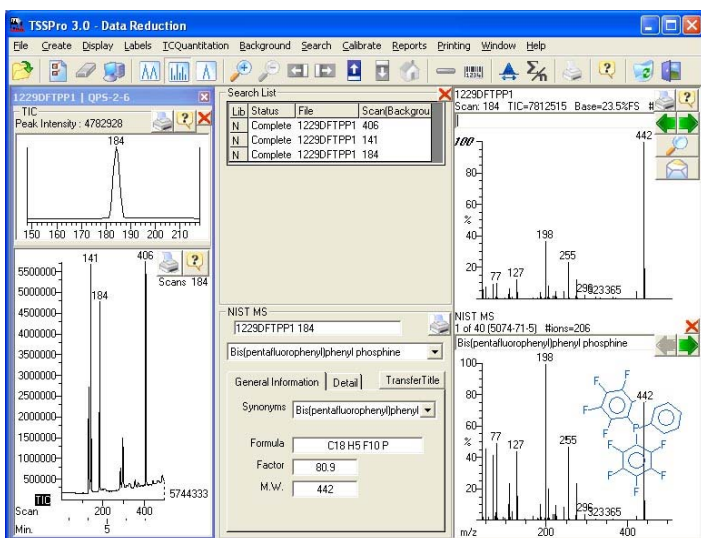
On-line help system guides you through the system with description and examples to make the process of extracting your mass spectra as easy as possible.

Data Reduction Options

High Resolution/Accurate Mass

Recalibrate mass spectra with internal reference to determine accurate masses for unknown ions. These accurate masses are then used to calculate elemental compositions.

Possible compositions are calculated based on the elements and limits that you specify. Accuracy of the results are reported in ppm or mmu.



Results from a NIST library search

Library Searching

With a click of the mouse, start a library search into the NIST or Wiley database. Match factors, indicating the reliability of the match, and other information including formula molecular weight and structures are returned from the selected database. View the returned mass spectrum with its structure against the original unknown for visual

confirmation. Label the unknown mass spectrum with compound name and structure so later reviewing of data will display the saved name and structure. Automatic and multiple search capabilities allow for fast processing of unknowns.

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Specializing in Mass Spectrometry since 1971



Computer Requirements (Minimum)

- Pentium with mouse, CD-ROM and 32 Mbytes RAM
- Microsoft Windows 95 or greater
- 2 -3 expansion slots for interface boards (instrument dependent)
- Super VGA Monitor 800x600
- Printer compatible with installed version of Windows

Interface Hardware

- Conversion speeds of 333kHz/s
- 2 16-bit A/D converters
- 2 16-bit D/A converters
- Input / Output Signal: 0 - 10 Volts

New Features

New features are being added daily so contact your local representative with specific questions.

Special Applications

Shrader Laboratories is available for customizing this software or developing new software to meet your needs. Manufacturer and single-user projects are welcome and kept confidential.

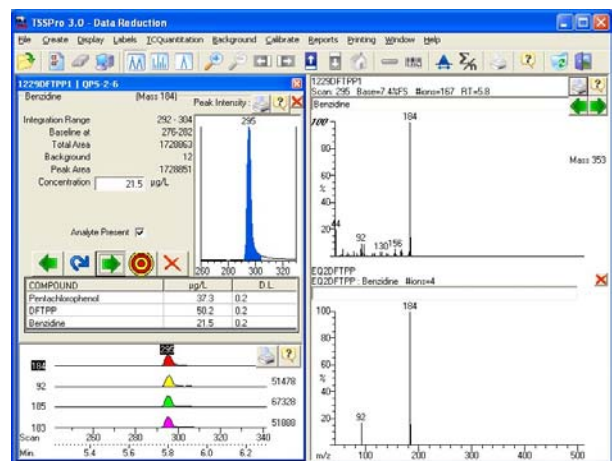
More Data Reduction Options

Target Compound Quantitation

A reverse-search is performed on an unknown sample for compounds entered into a user generated list. A report with concentrations and detection limits is generated.

The combination of selected ion

monitoring and target compound quantitation gives ultra-high sensitivity, detection and measurement of selected target compounds. Target compound lists may be created with up to 200 internal standards and/or compounds of interest.

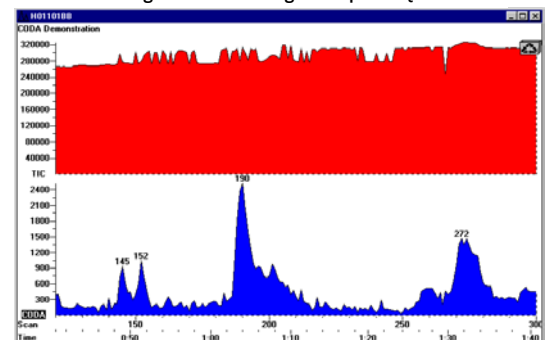


Viewing the results of Target Compound Quantitation

CODA

Component Detection Algorithm (CODA) creates mass chromatograms for every mass over a specified range, then detects those masses that are chemically significant. Those masses can either be combined to create a CODA TIC or displayed individually to resolve compounds that coelute. CODA

is perfect for reviewing LC/MS data where the TIC is almost useless and GC/MS where several compounds coelute and form a single peak in the TIC.



A useless TIC compared to a CODA TIC