

Expert™ Software

# Sulfur Expert™

Simplify your 'data to decision' workflow

**Sulfur Expert™** greatly simplifies your ability to review and characterize sulfur speciation (GC) data as well as manage it. Calibrate your GC using a sulfur component library that can be easily updated and expanded as compounds are identified. Sulfur data can be quantified by individual component, by organo-sulfur group, as a composite or by a calculated physical property you specify. And, with the built in peak integrator, you can do all of your work in single software environment.

Group	[PPM](w/w)	Sulfur [PPM](w/w)
Mercaptans	38.72	2.54
Thiophene	0.00	0.00
C1 Thiophenes	27.24	6.72
Tetrahydrothiophene	0.00	0.00
C2 Thiophenes	43.55	7.14
C3 Thiophenes	48.57	0.30
C4 Thiophenes-2	18.38	0.77
Unidentified-1	37.76	N/A
Benzothiophene	0.00	0.00
+ Benzothiophene-1	6.50	0.24
C4 Thiophenes-1	26.79	2.61
Unidentified-2	10.95	1.41
<b>Total</b>	<b>258.46</b>	<b>21.74</b>

Sample Id: 13513-1 Sample File: 13513-1\_AED3\_A

### Total Concentration or Sulfur Concentration

Results are reported as total concentration of the component and the concentration directly attributable to the sulfur content itself.

### Organize Components by Group

User can create sulfur groups ex. thiols, sulfide, disulfide, isothiocyanate, thiophene etc.

Concentration Units: PPM

Precision: Time 3, Other 2

Component Groups:

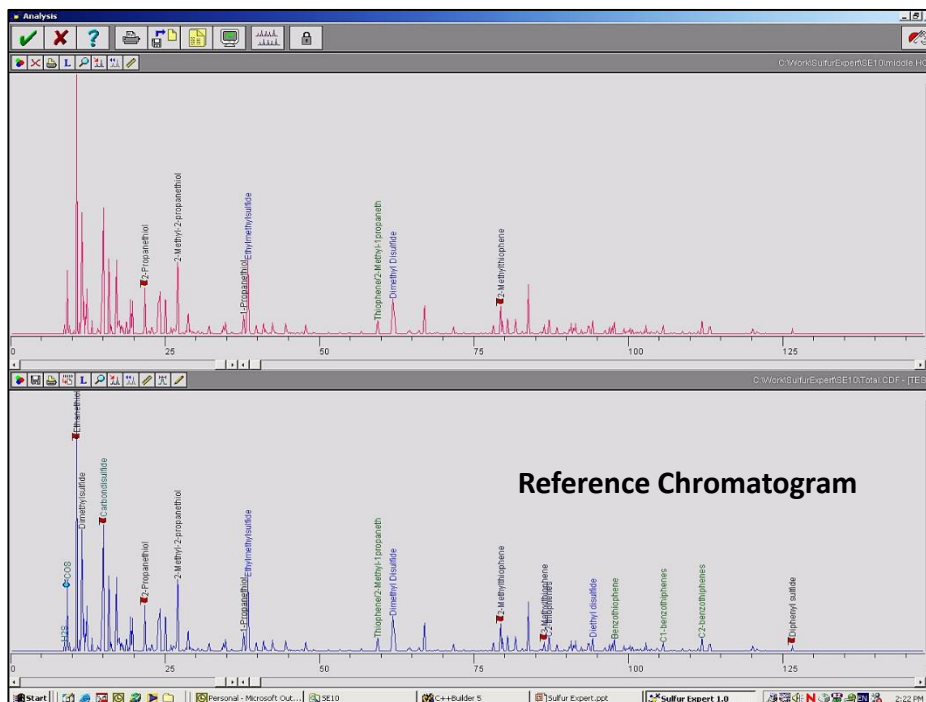
Code	Name	Color	Type
M	Mercaptans	Black	Mercaptans

Buttons: OK, Help, Cancel

# Software Highlights

## Simplify Peak Identification

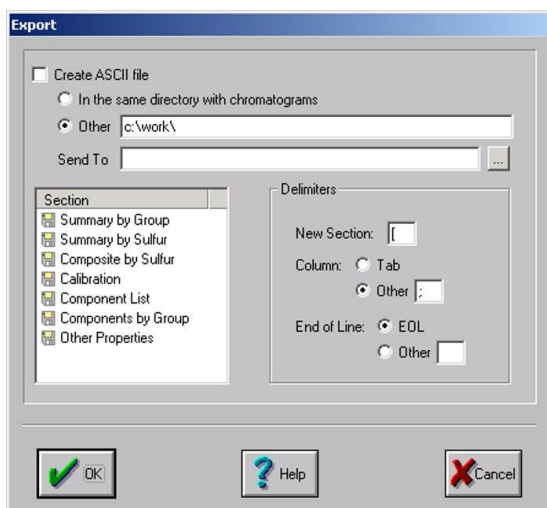
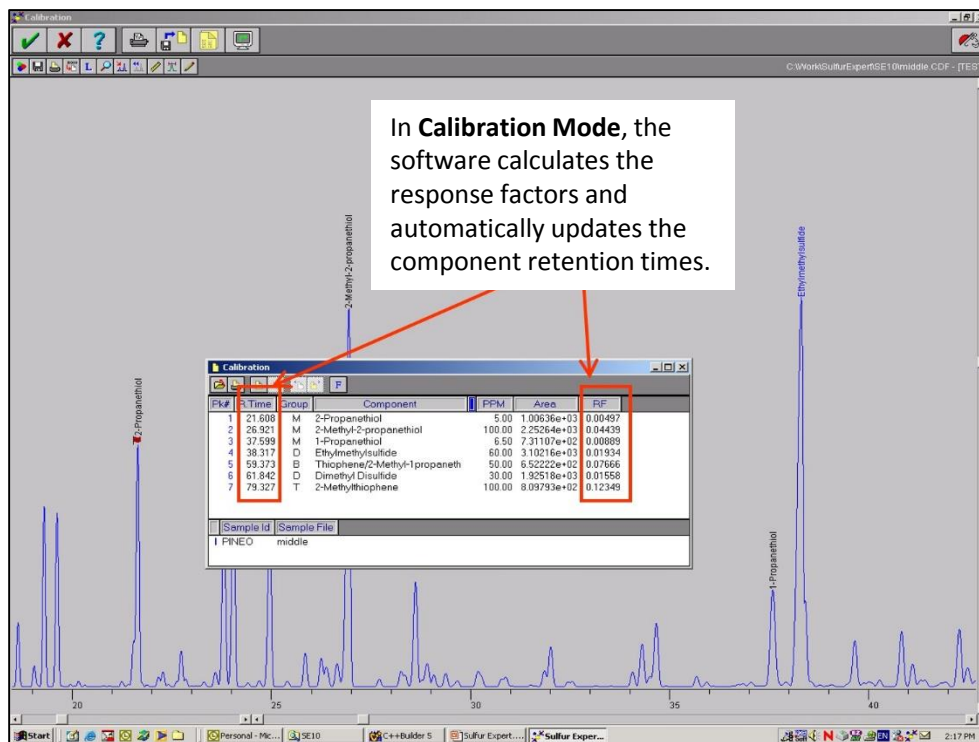
Reference chromatograms can be displayed on screen to help identify unknown peaks. There's no need to type in a retention time once a peak has been identified. It only takes a couple of mouse clicks to change a peak's identification.



Summary by Group						
Group	[PPM](w/w)	Sulfur [PPM](w/w)	[PPM](w/w)	Sulfur [PPM](w/w)	Diff	Diff
Mercaptans	38.72	2.06	38.72	2.06	0.00	0.00
Thiophene	0.00	0.00	0.00	0.00	0.00	0.00
C1 Thiophenes	36.09	0.28	27.24	6.24	8.85	-5.96
Tetrahydrothiophene	3.69	0.85	0.00	0.00	3.69	0.85
C2 Thiophenes	14.59	2.56	43.55	6.19	-28.97	-3.64
C3 Thiophenes	0.00	0.00	48.57	0.28	-48.57	-0.28
C4 Thiophenes-2	18.38	0.62	18.38	0.62	0.00	0.00
Unidentified-1	171.43	N/A	37.76	N/A	133.67	N/A
Benzothiophene	0.00	0.00	0.00	0.00	0.00	0.00
+ Benzothiophene-1	6.50	0.21	6.50	0.21	0.00	0.00
C4 Thiophenes-1	26.79	2.43	26.79	2.43	0.00	0.00
Unidentified-2	10.95	1.23	10.95	1.23	0.00	0.00
327.14 10.23 258.46 19.26						
Sample Id	Sample File					
+ IC13513-1	13513-1_AED3_A					
+ IC13513-1	13513-1_AED3_A					

Results from 2 or more analyses can be compared.

## Software Highlights



### Easily Share Results

Results can be exported as ASCII delimited files. These files can be imported into applications such as LIMS, Excel, etc.

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# Software Capabilities Summary

- There are two basic modes of operation; calibration and analysis
  - **Calibration mode**
    - Response factors are calculated using the peak areas and amounts of individual components (derived from information contained in the identification table prepared and maintained by the user) and the component retention times are updated accordingly.
    - Due to the challenge to obtain commercial gravimetric standards that include all of the compounds of interest, calibration can be performed in multiple steps over time using different standards (as long as each standard used contains different components).
    - User can organize the sulfur components into various organo-sulfur groups (ex. thiols, sulfide, disulfide, isothiocyanate, thiosulfinate, thiophene etc.) in the identification table and specify color coding to make it easier to visually identify one group from another.
    - An unlimited number of components can be added to the groups
    - Concentrations can be in terms of w/W, v/V or m/M
  - **Analysis mode**
    - Components are identified and reported in elution order
    - All results can be viewed and compared on screen and visibly differentiated via color coding
    - Concentration results can be reported by group, sulfur composite, individual component, component list by group and calculated physical properties
    - Reference chromatograms can be recalled and viewed on screen to facilitate identification of unknowns
    - User defined calculations can be added and performed
    - Results from multiple samples can be compared on screen
    - Results/reports can be exported as ASCII delimited files which can then be sent onto a LIMS or imported by MS Excel
- A built in peak integrator negates the need to acquire the detector signal via data acquisition software such as ChemStation or OpenLab first before processing it; this saves time and reduces operational complexity
- Utilizes a highly intuitive, graphical user interface
- Compatible with all of the popular (GC) chromatography data acquisition software platforms including: ChemStation, OpenLab, Chromeleon, XCalibur, TurboChrom, Compass and others.

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