



Food & Flavour Analysis by PFPD

Introduction

- Sulphur compounds are an important component of flavour analysis
- Responsible for specific and distinctive flavours in many foods & beverages
- Difficult to analyse and identify because present at minimal concentrations
- MS or FID commonly used, but not sensitive enough to detect sulphur compounds at trace levels

GC Configuration MS/FID/PFPD



Agilent FID in Front
for Sulphur Marking

OI Analytical PFPD in Back
For Quantitation

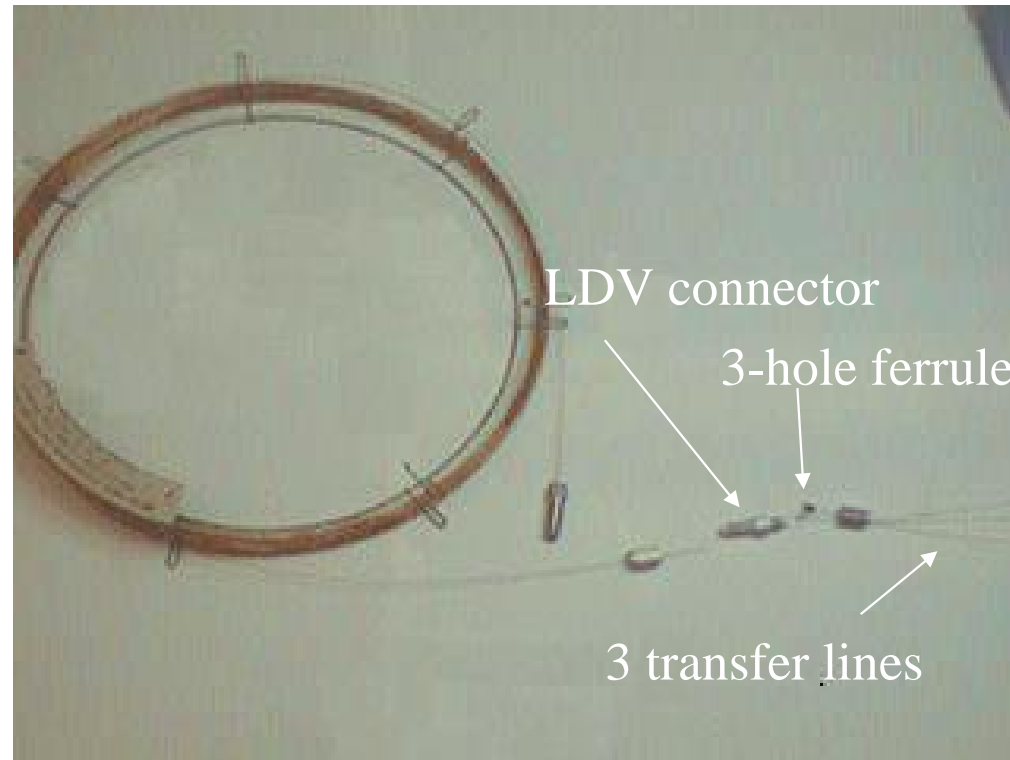
6890N GC with
5973N MS



Column Configuration for 3 Detectors



Standard installation
at injection port



Detector end split using low dead volume
connector and a 3-hole ferrule

Headspace Apparatus



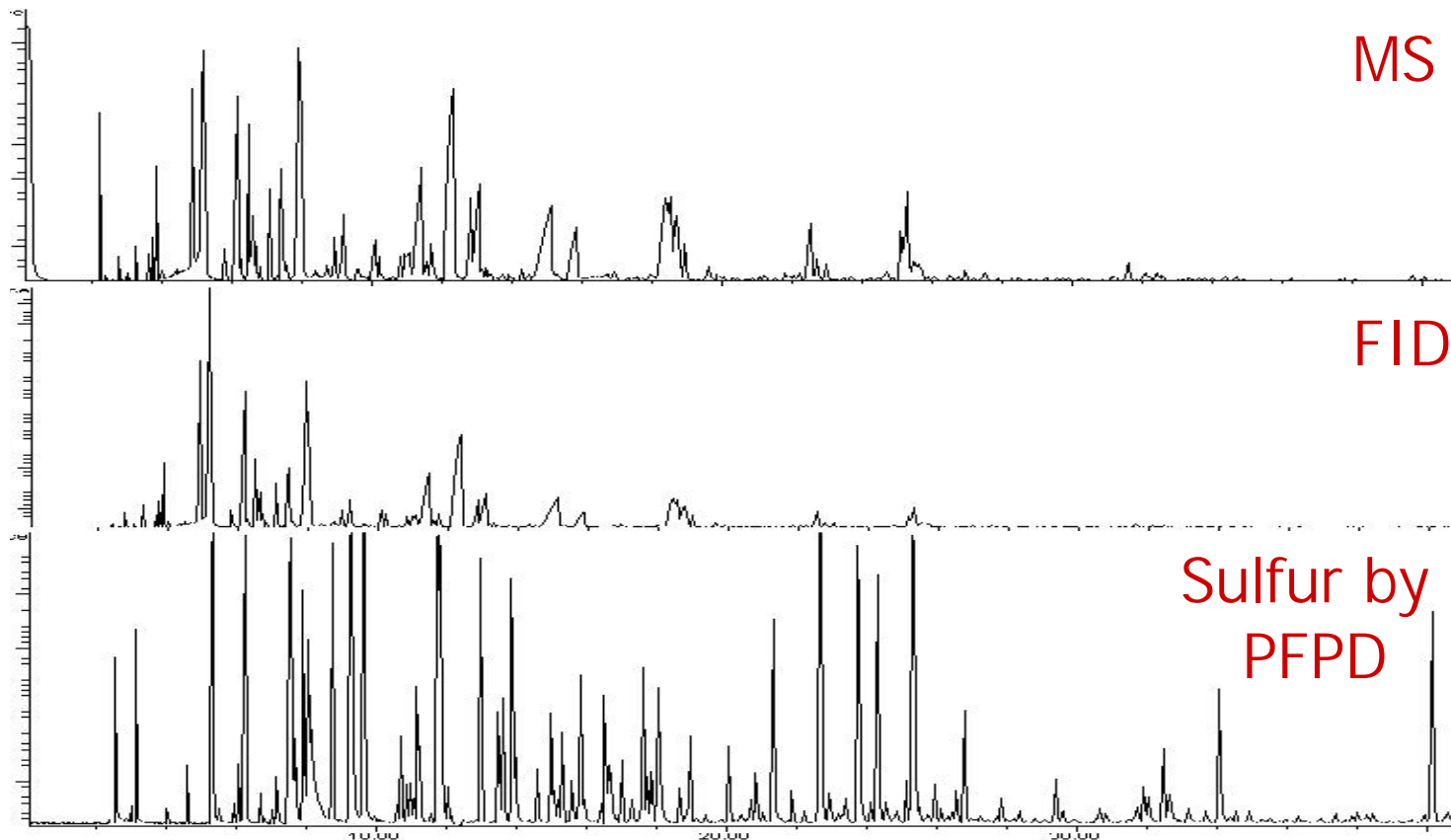
Line carrying He
purge gas

GC inlet liner packed
With 100 mg Tenax

~20 grams coffee

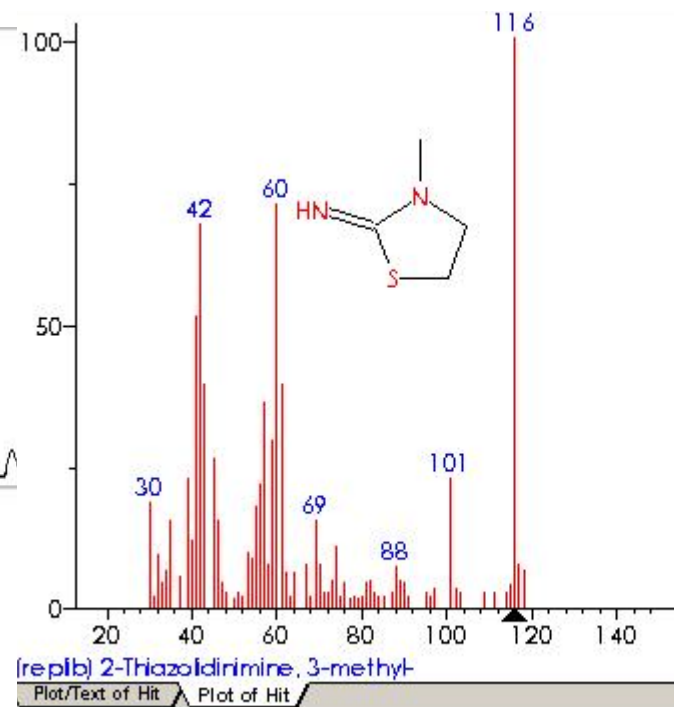
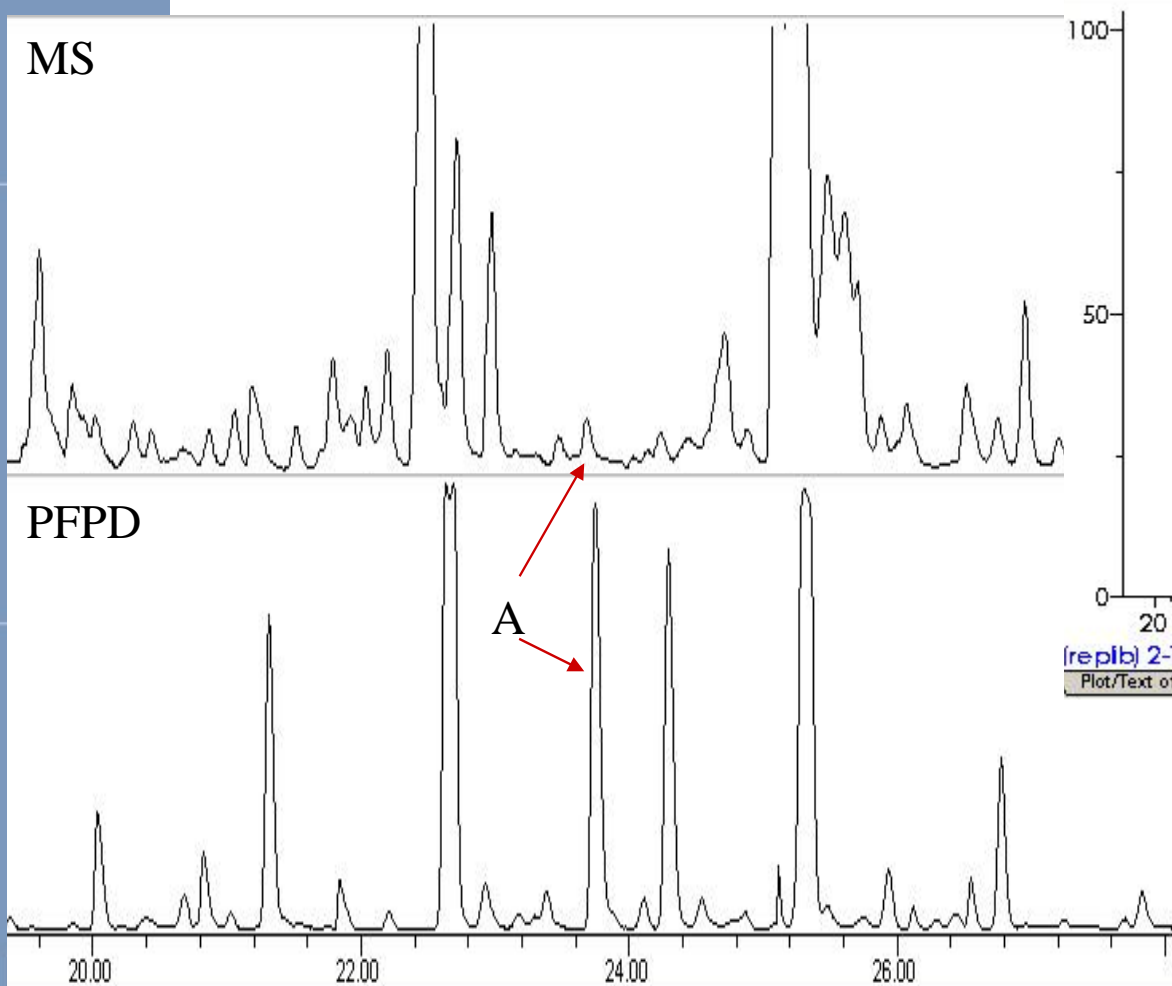
Coffee Headspace by MS/FID/PFPD

3 Simultaneous Chromatograms From Coffee "A"



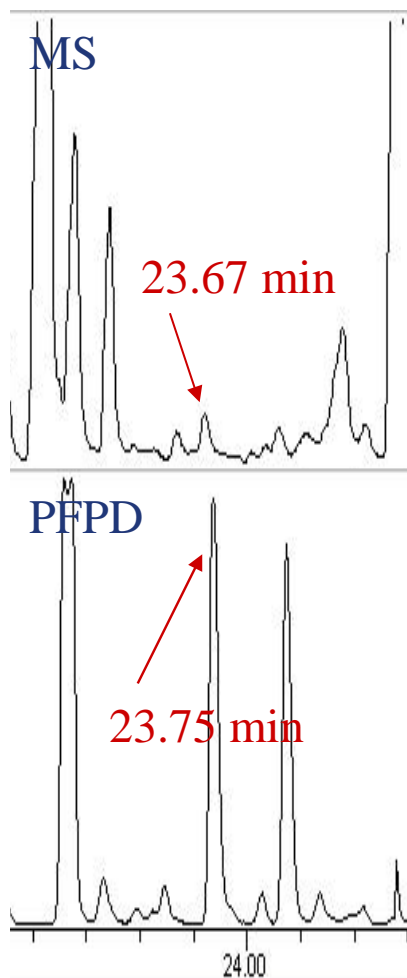
Over 200 sulfur peaks detected

PFPD Used To Identify Sulfur RTs



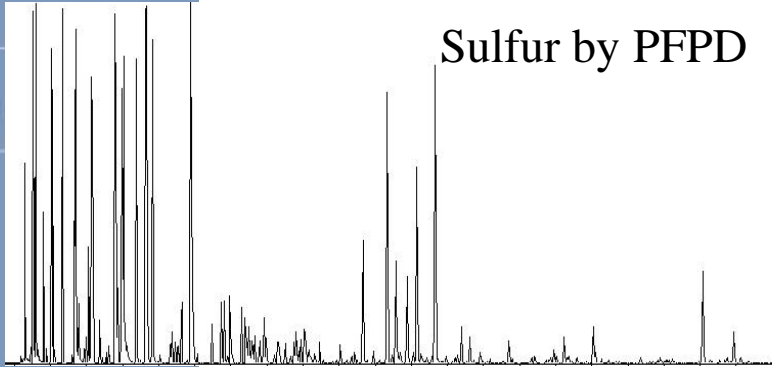
NIST search results
for peak "A"

Compound Retention Times



- MS and PFPD (and FID) chromatograms very slightly offset by 4-5 seconds
 - Reproducible
- Due to fact that MS is under vacuum and PFPD and FID are under slightly positive pressure
- Offset easily determined with a standard prior to analysis of unknowns

Competitive Analysis

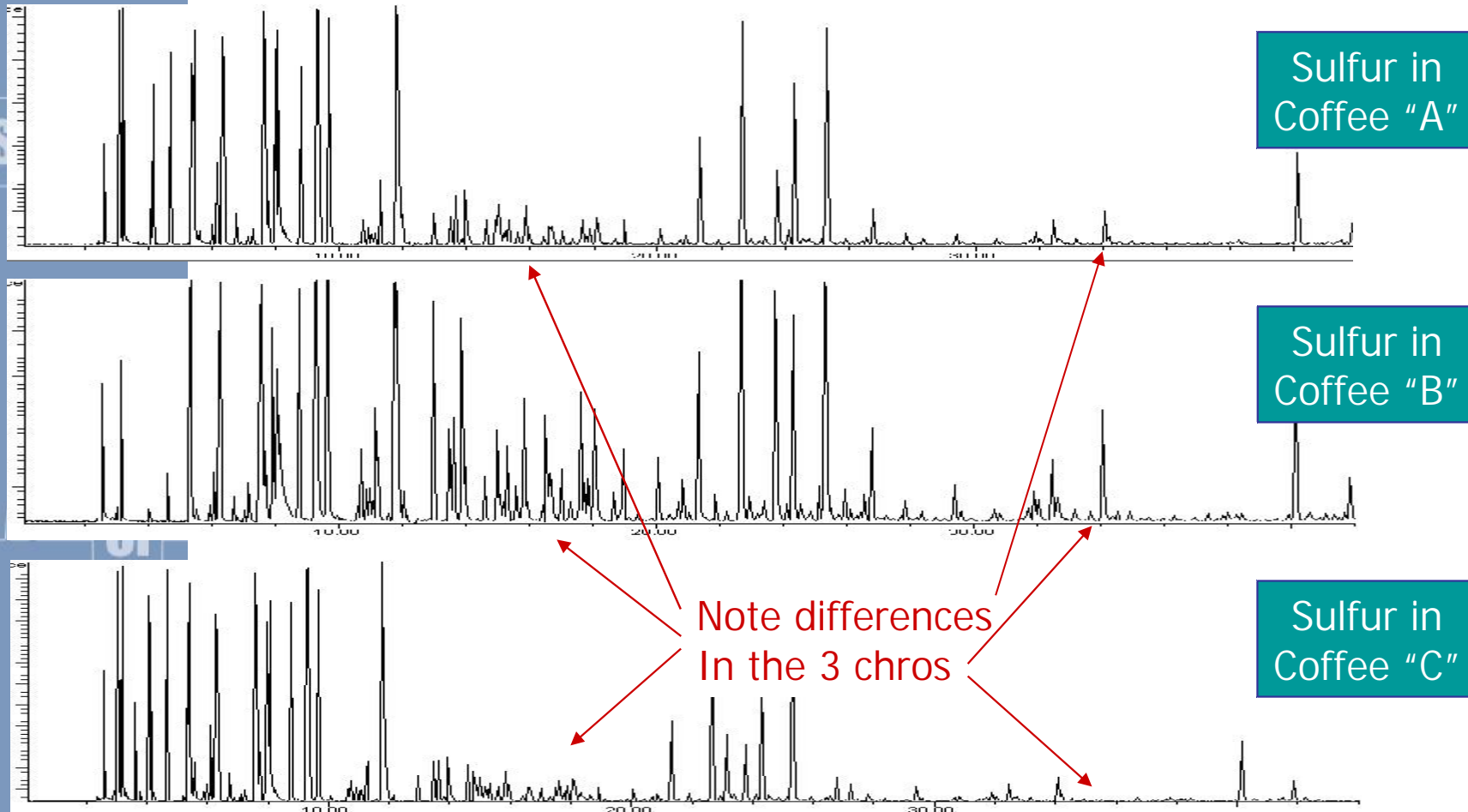


Sulfur by PFPD

- The sulfur chromatogram, or “fingerprint” is unique for each coffee blend

- Can be used to identify differences between specific blends
- Determine which sulfur compounds contribute distinctive flavor and aroma

Competitive Analysis of 3 Coffees



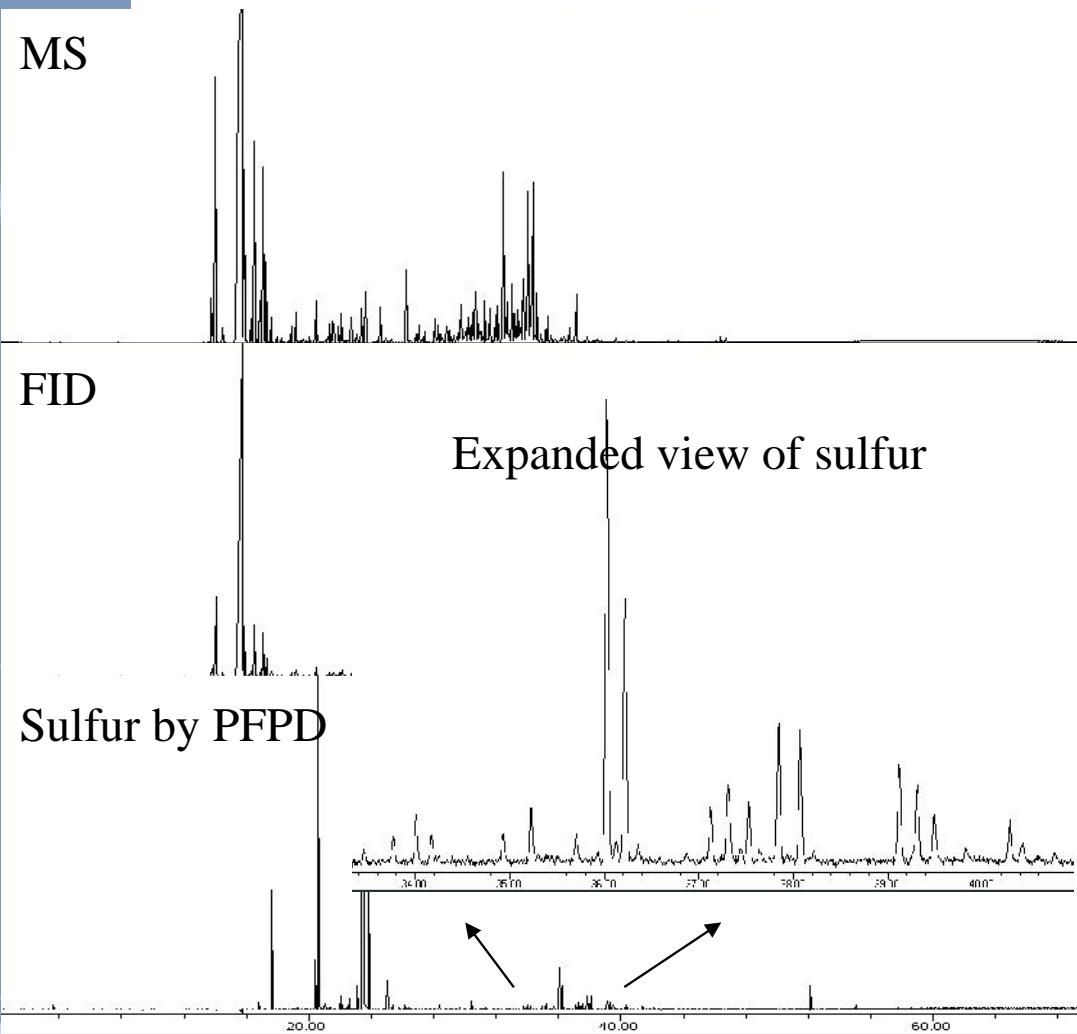
Sulfur in
Coffee "A"

Sulfur in
Coffee "B"

Sulfur in
Coffee "C"

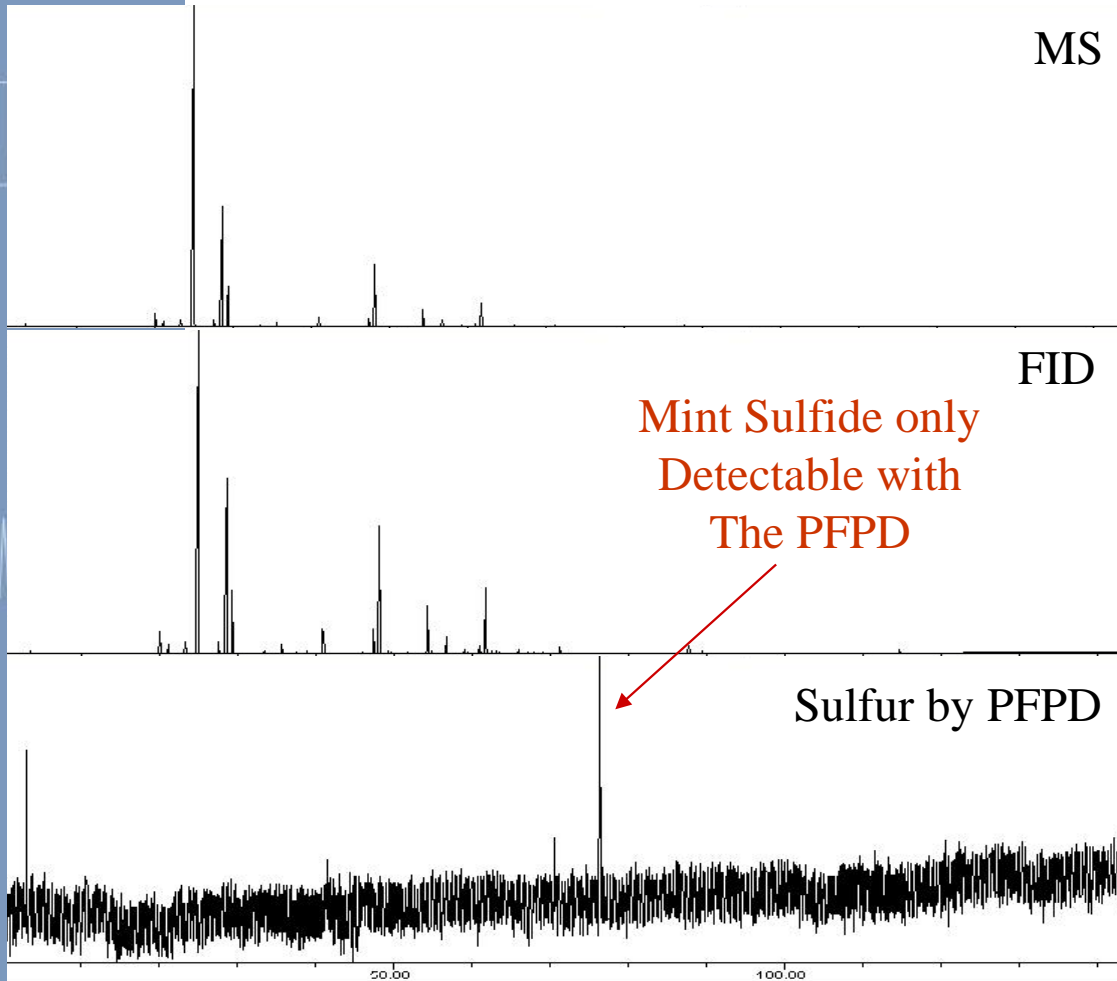
Note differences
In the 3 chros

Sulfur in Galbanum Oil by PFPD



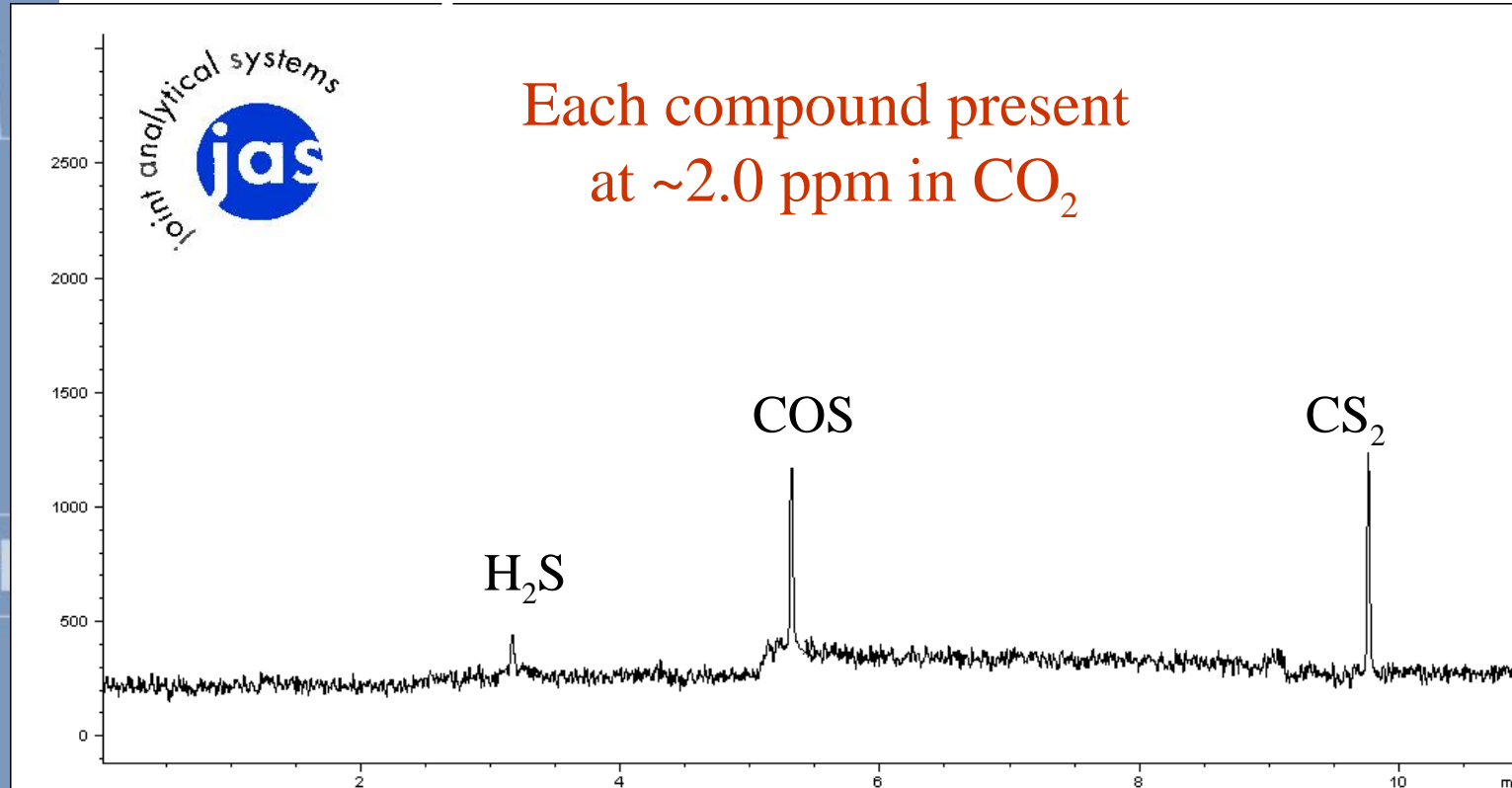
- Essential oil distilled from the galbanum plant
- Green, fresh leafy odor, dry woody undertones, pine highlights
- Used in production of fragrances
- Using an FPD only 4 sulfur peaks were detected

Sulfur in Fishwort Oil



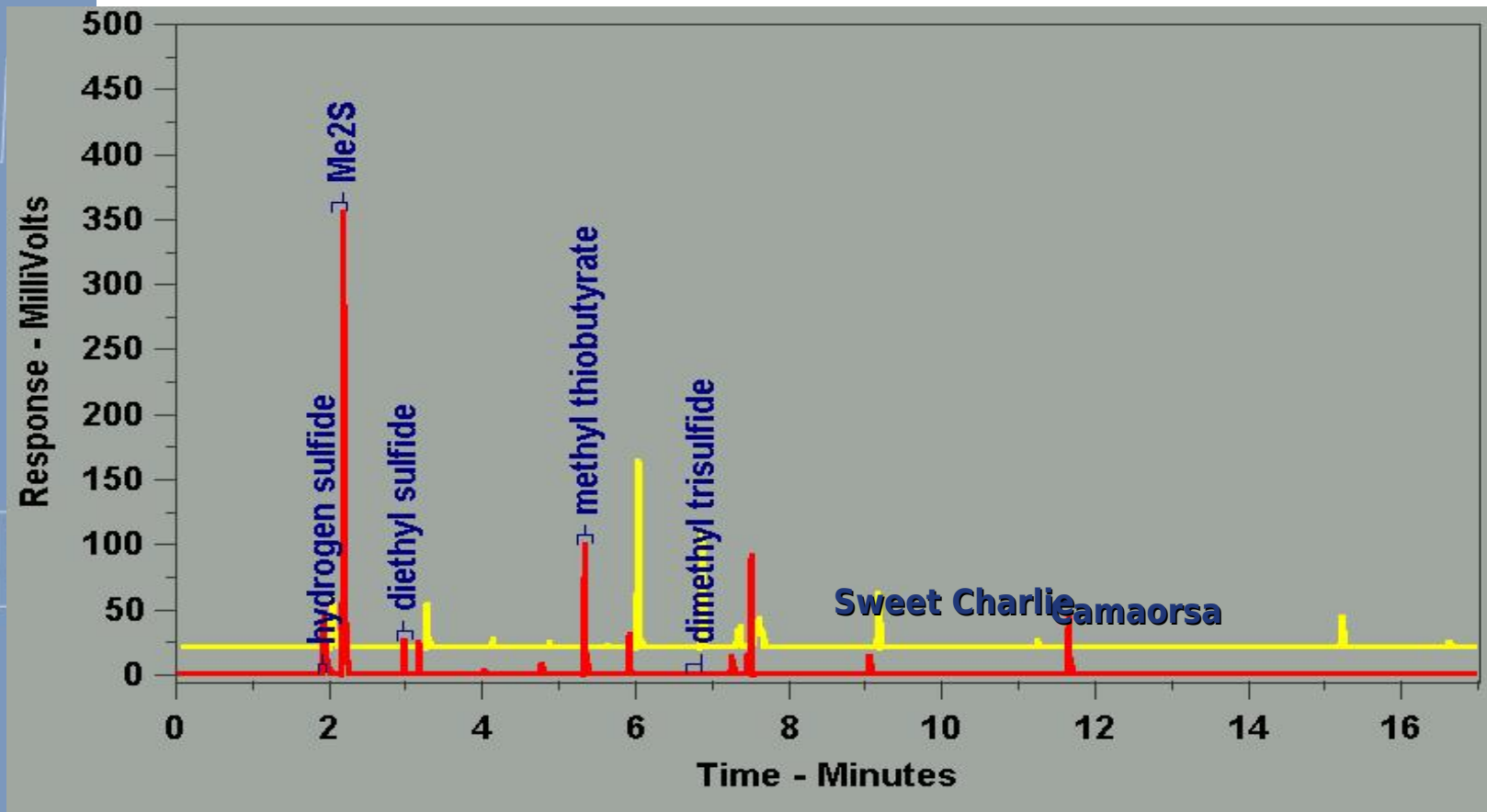
- MS • 0.1 μL injection
- Essential oil distilled from the fishwort, or “Chinese Lizard Tail”, plant (2 varieties)
- FID • Corriander aroma or lemon/orange odor
- Used in production of flavors
- Using an FPD no sulfur peaks were detected

Sulfur in Beverage Grade CO₂



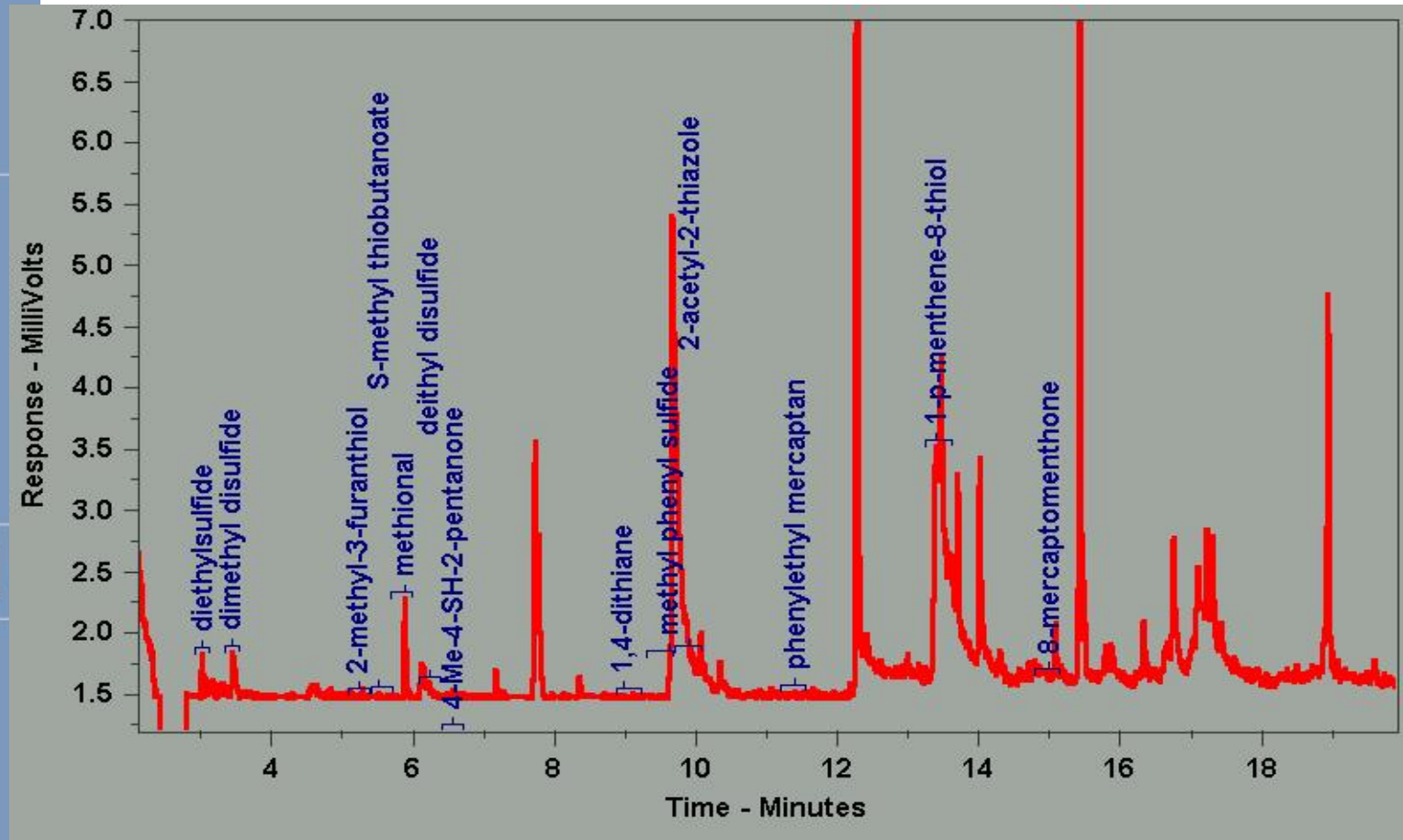
Chromatogram courtesy of JAS

Sulfur in Strawberry by PFPD



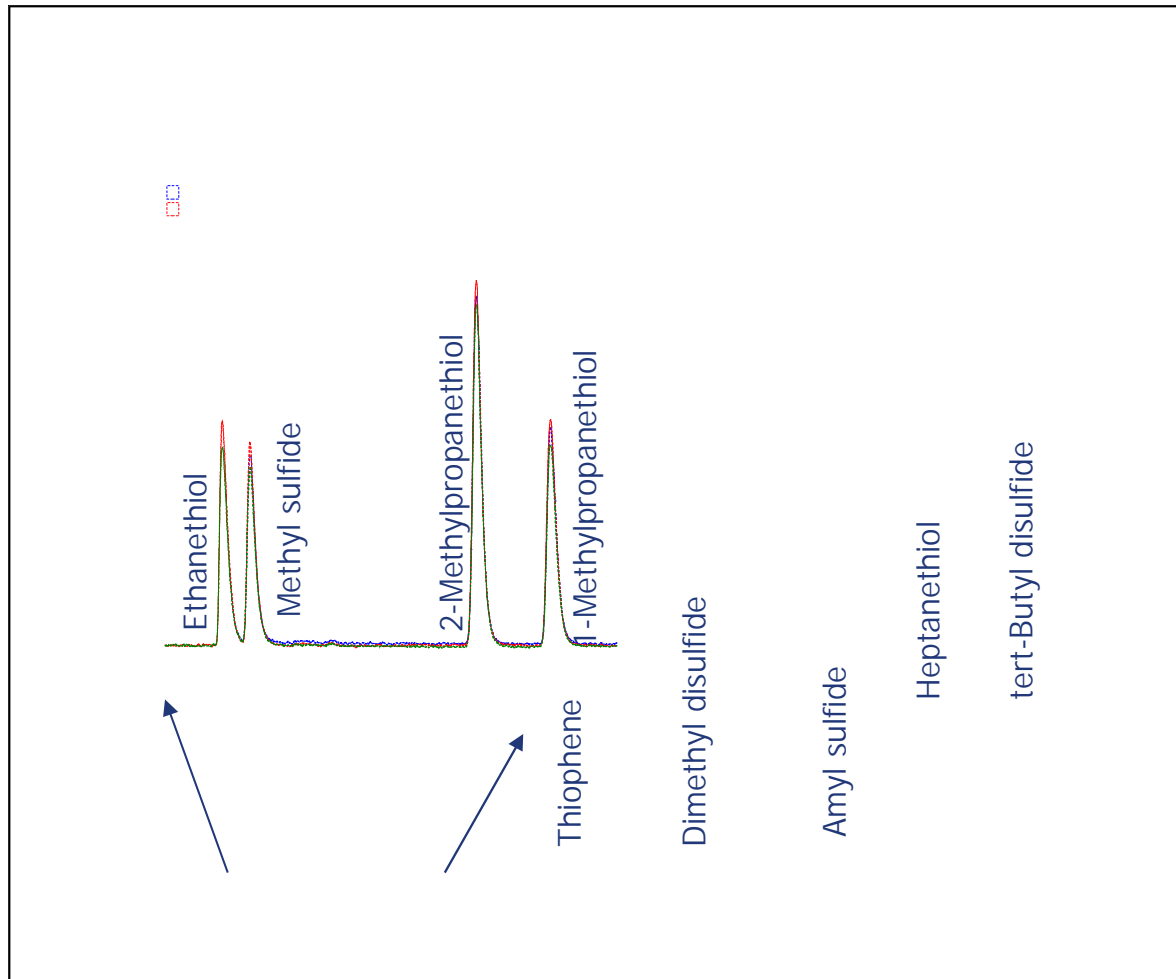
Chromatogram courtesy of Russell Rouseff, PhD, at University of Florida

Sulfur in Grapefruit by PFPD



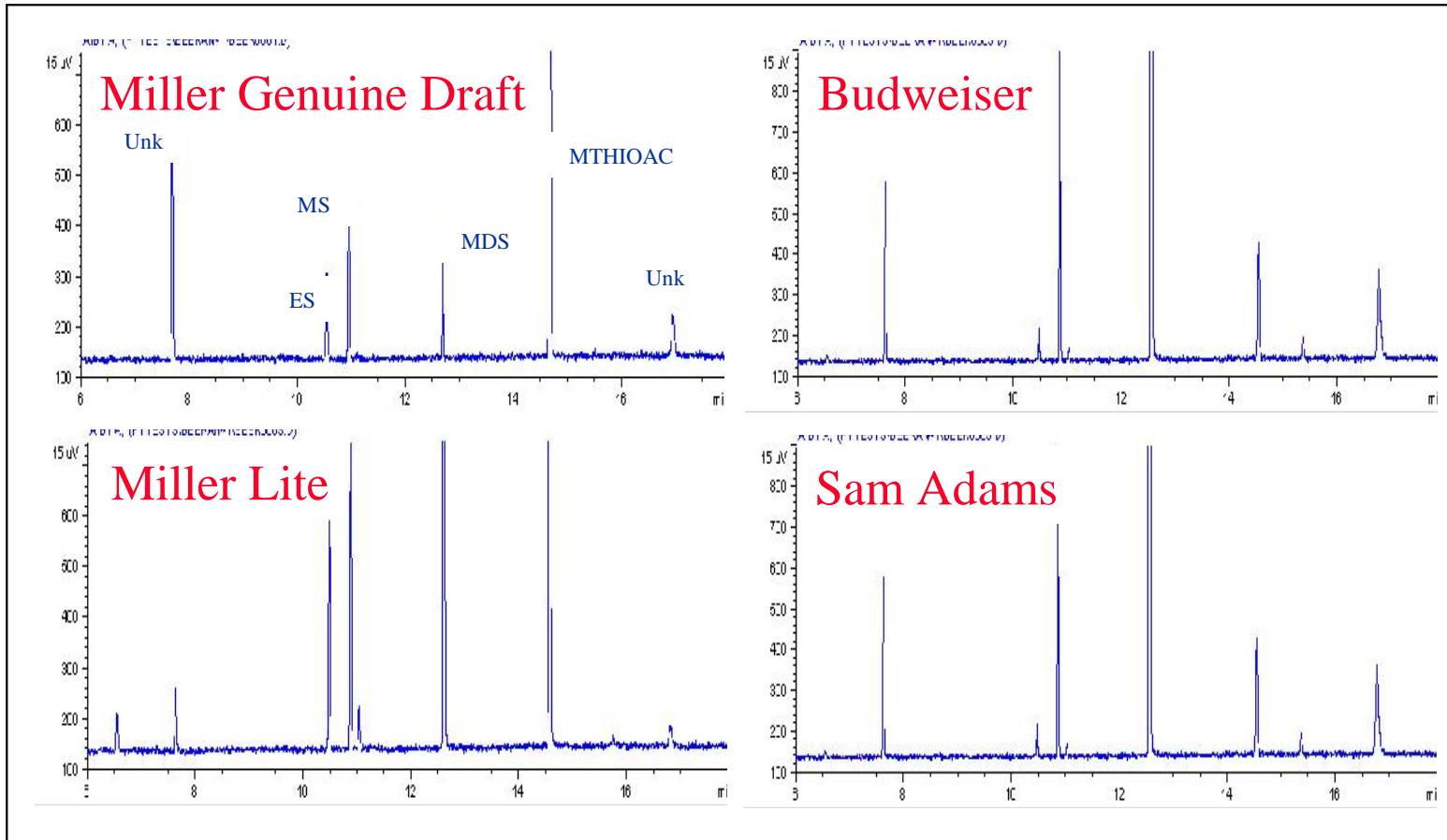
Chromatogram courtesy of Russell Rouseff, PhD, at University of Florida

Sulfur in Beer by Headspace



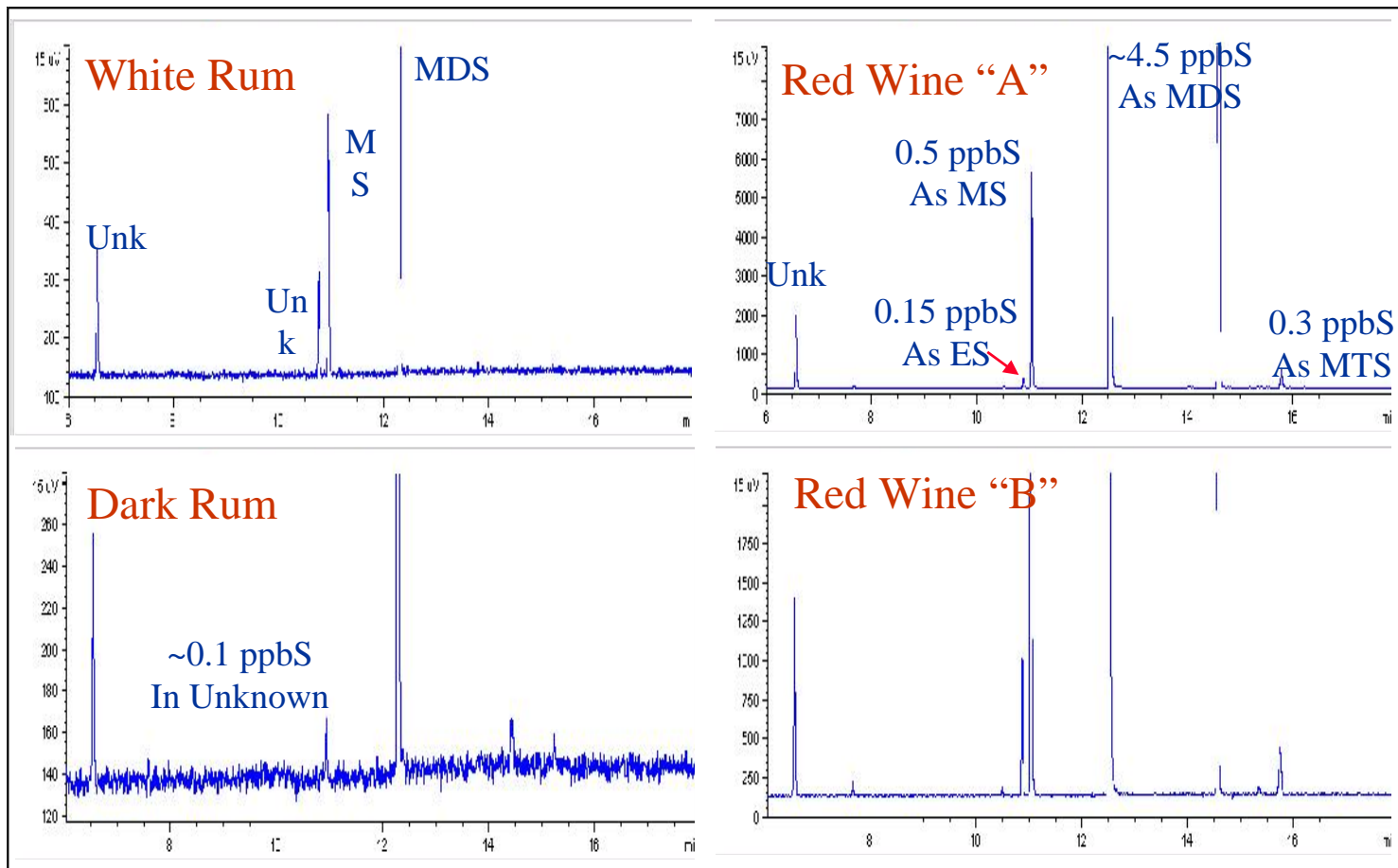
PFPD
repeatability
at 10 ppb
better than
10%

Sulfur in Beer by PFPD

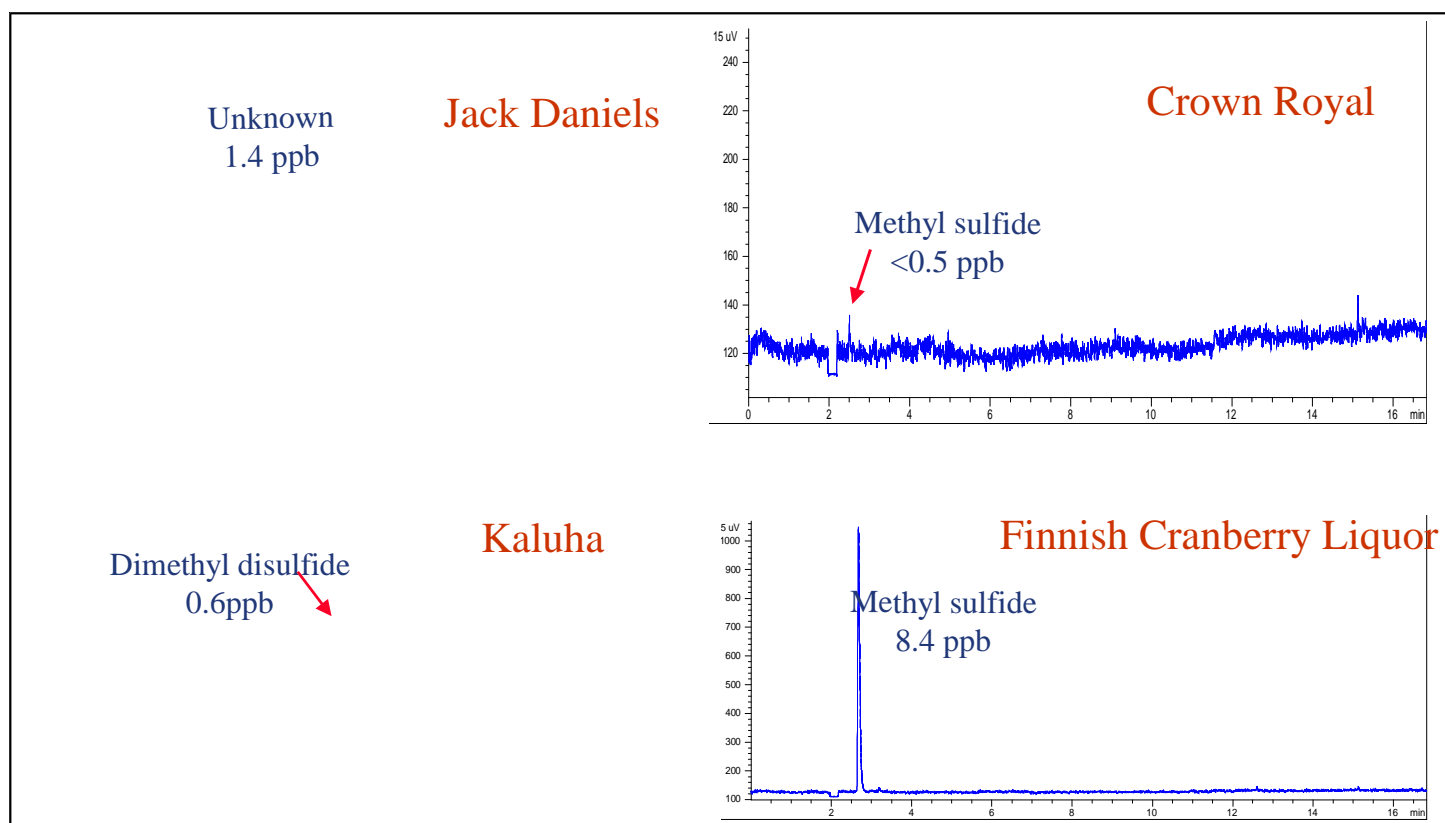


Sulfur concentrations in beers tested ranged from 0.1 ppbS to ~4 ppbS

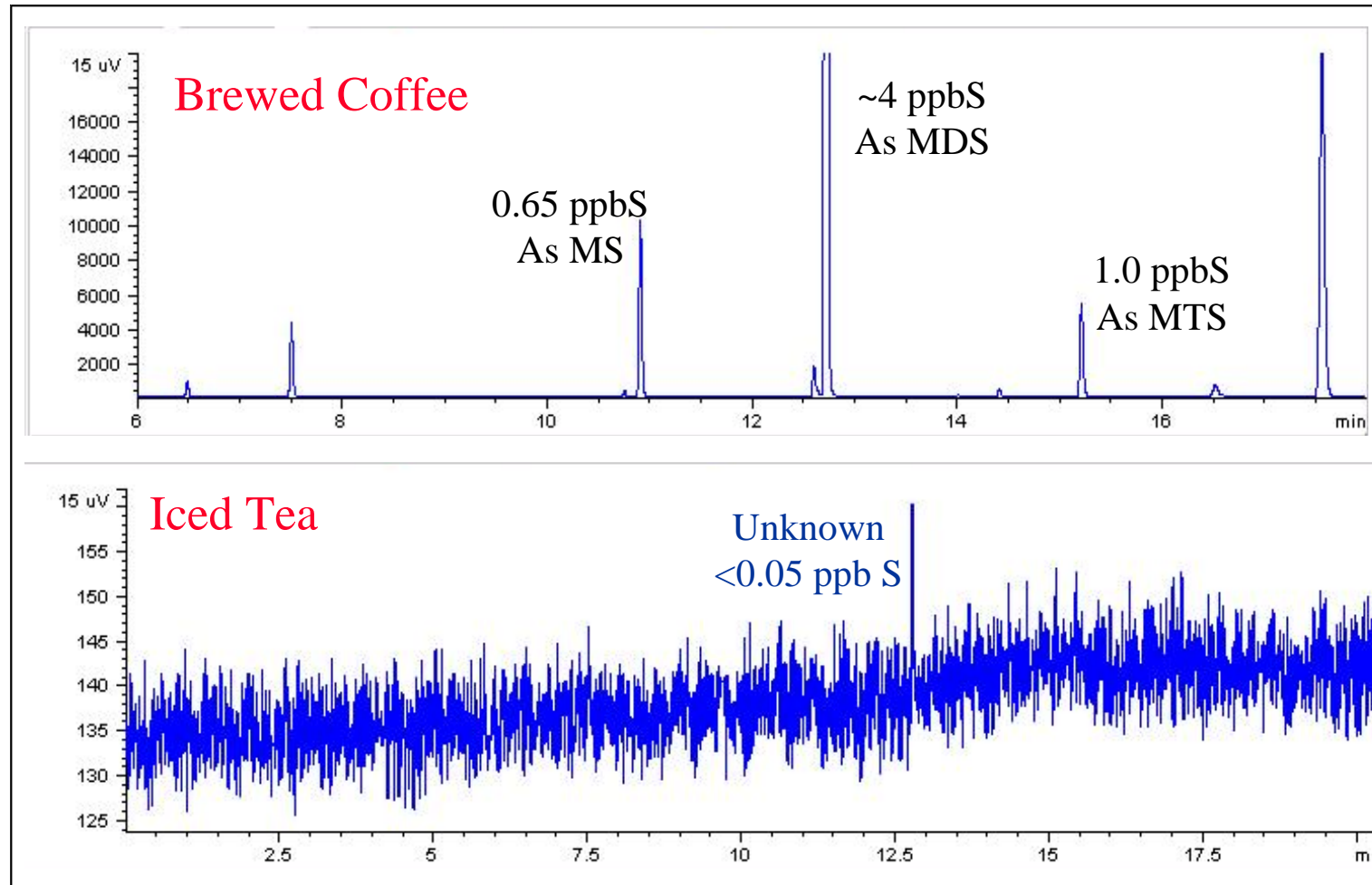
Sulfur in Wine and Rum by PFPD



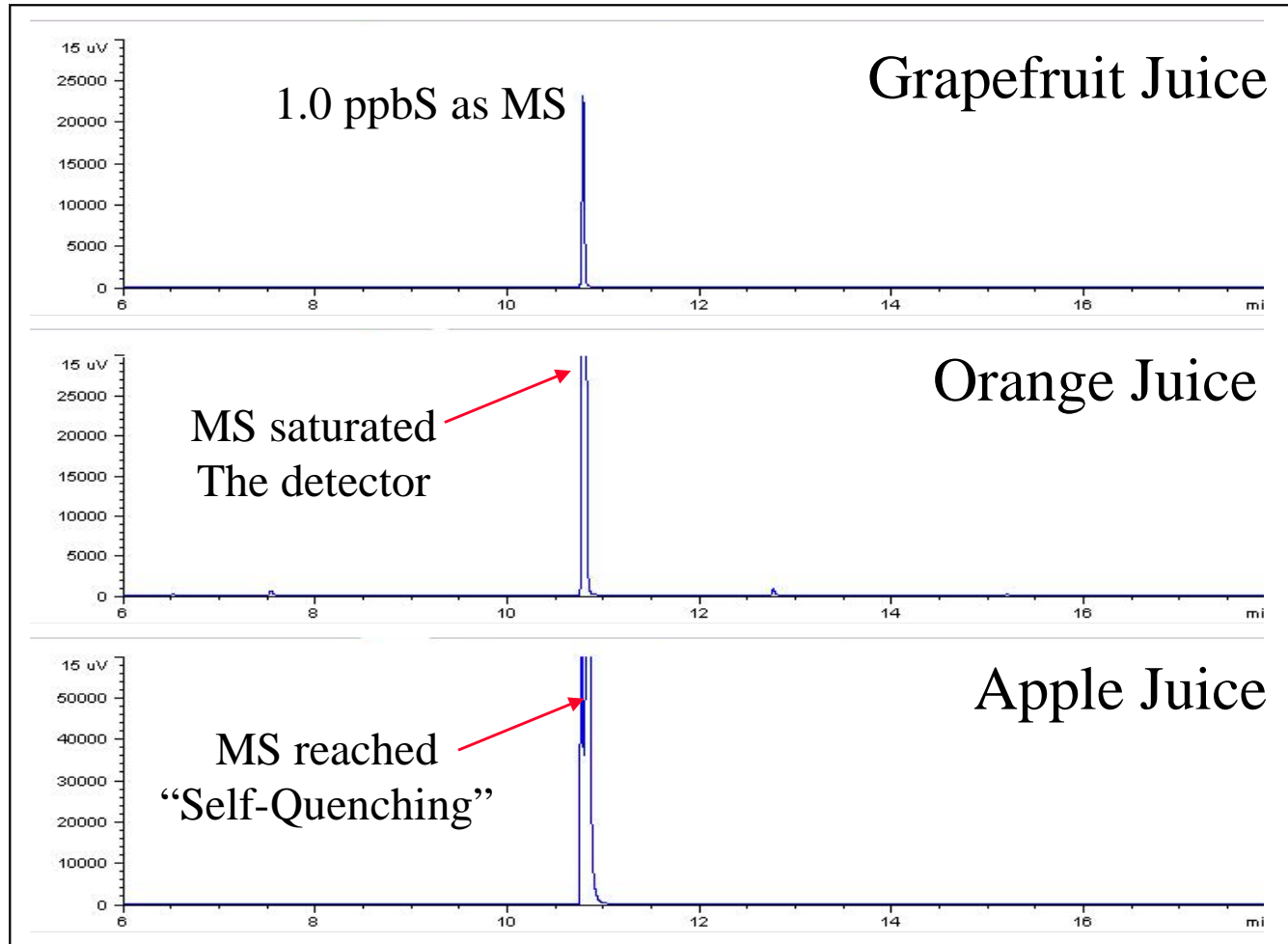
Sulfur in Liquor by PFPD



Sulfur in Coffee & Tea by P&T/PFPD



Sulfur in Juice by P&T/PFPD



PFPD-MS Configuration

