Matlab Application to Process GC-MS Data

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GCMS Process

- An unknown sample mixture is injected onto the gas chromatograph where it is vaporized
- The mixture components separate as they travel through a long, coated silica capillary
- Components then pass into a mass spectrometer where they are ionized, fragmented, and detected

Why use GCMS data

- Each mixture component is fragmented uniquely by the mass spectrometer
- Information can be used to identify compounds or compare samples
- Quantitatively measures subtle differences
- Can be used for characterizing complicated mixtures such as fuel

Application Goals

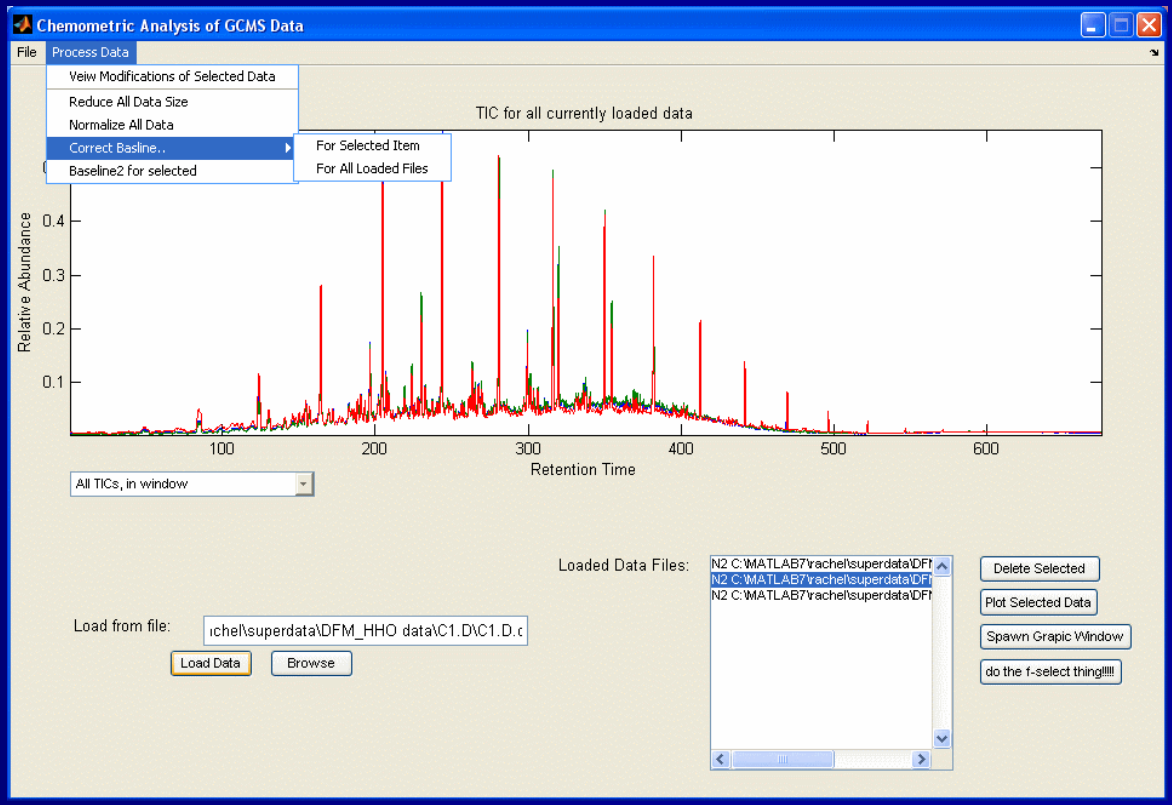
- GC-MS Data needs to be analyzed to yield information
- Tools need to be accessible to chemists, even those unfamiliar with computer science
- Program should be flexible, to allow changes as new tools are developed

Issues

- GC-MS data sets are large and difficult to view manually
- Should be easy to use – this means no command prompts
- Needs unified data format
- Hard to communicate between separate programs

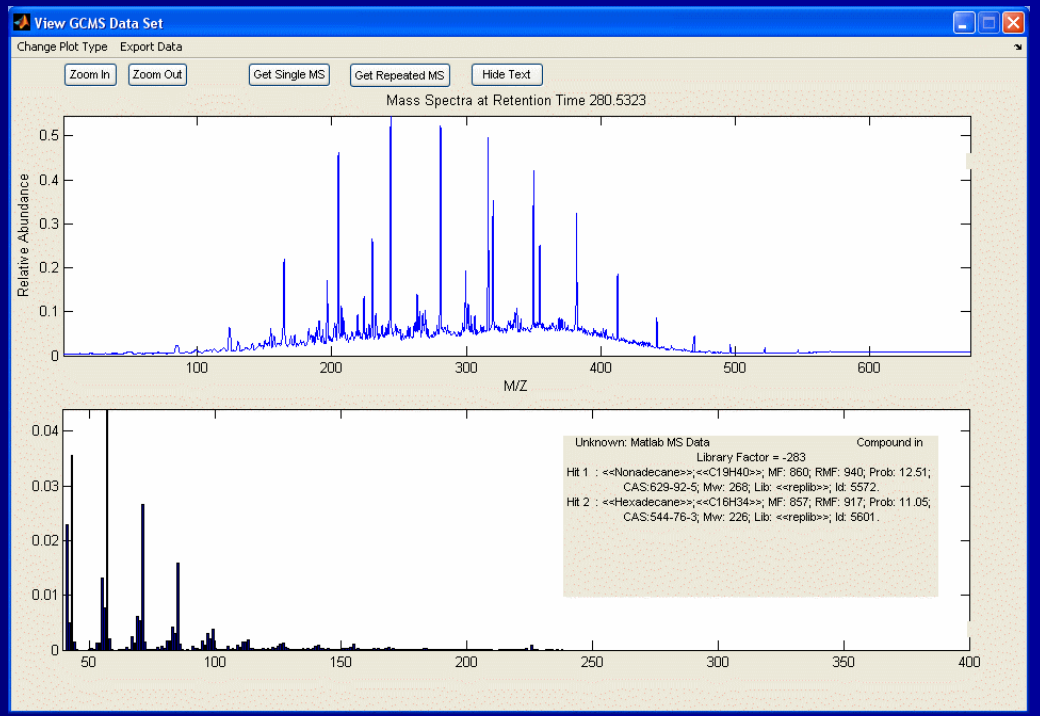
Introduction to GC-MS Application

- Program uses multiple clickable GUIs
- Once data is loaded, user makes new windows for different jobs
- Data may be viewed, processed, or analyzed



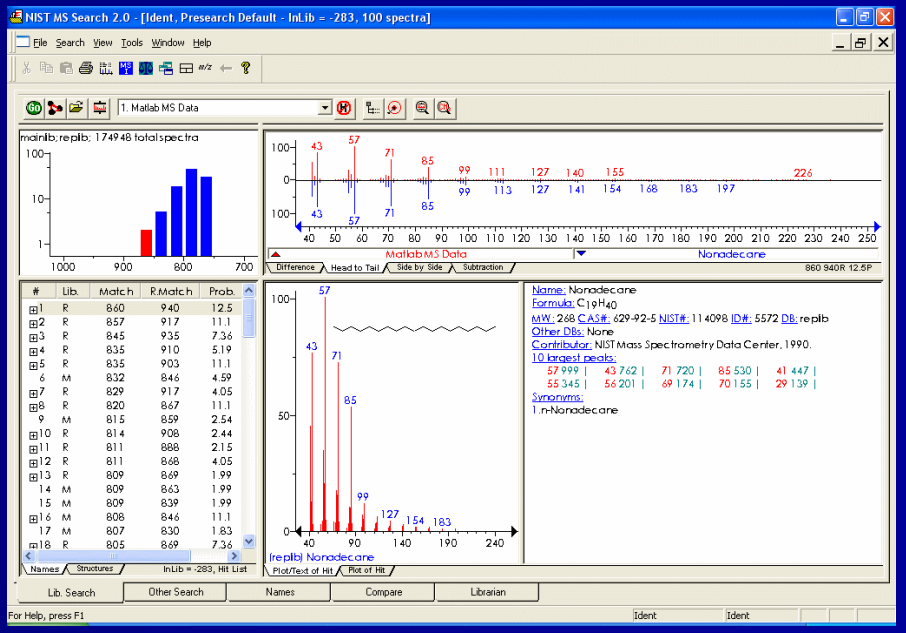
View graphics

- Data may be viewed as a whole, Total Ion Chromatogram, Single Ion Chromatogram, or Mass Spectra
- Graphs respond to user interaction – clicking, adjust contrast..
- Can be used to compare graphs or for more information



NIST Mass Spectra Search

- Mass Spectra may be sent to NIST database
- NIST returns most probable compound
- Useful for identifying components of samples



Analyzing Data

- ANOVA - ANalysis of VAriance used on data sets
- Feature Selection keeps the most different parts of each plot
- Chemometric tools – factor analysis, helps find additives or components that are mixtures

Easily expandable in future

- Employs single, consistent data structure
- Modular nature – easy to add new GUI or new functions
- Important as new tools are developed, or are needed

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