

# Analysis of a Jet Fuel Standard using the TruTOF<sup>®</sup> HT TOFMS

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Key Words: TOFMS, GC, Chemical Ionization, Petroleum

## 1. Introduction

Time-of-Flight Mass Spectrometry (TOFMS) using an Electron Ionization (EI) source produces spectra with reproducible fragmentation patterns that can be automatically compared against standard libraries for analyte identification. Through the use of Chemical Ionization (CI), fragmentation is minimized and a strong molecular ion signal is observed. These two ionization methods are complimentary and allow for the determination of structure (EI) and molecular weight (CI).

In this study we show the analysis of a standard jet fuel standard under both EI and CI (positive ion) conditions. Structural characteristics revealed by the EI spectra, combined with molecular ion determination seen in the CI spectra aid in overall analyte identification. These experiments were done on the TruTOF HT system which features easily interchangeable ion sources that are isolated from the mass analyzer. This system allows for the selective venting of the ion source chamber while keeping the mass analyzer under vacuum. This feature decreases instrument down-time when changing ion sources and allows for more samples to be analyzed over a short period of time.

## 2. Experimental Conditions

Sample: Jet Fuel Standard (Restek)  
Autosampler: Gerstel MPS2  
Syringe Type: 10  $\mu$ L syringe  
Injection: 1  $\mu$ L (splitless)

GC: Agilent 7890 Gas Chromatograph  
Column:

Rtx-5 (10 m x 0.18 mm i.d. x 0.20  $\mu$ m d.f.) MACH  
Oven:

40°C (3 minutes) to 300°C at 30°C/minute

Inlet Temperature: 250°C

Carrier Gas:

He at a constant flow of 1.5 mL/minute

MS Transfer Line: 275°C

MS: LECO TruTOF HT

ELECTRON IONIZATION at -70 eV

Acquired Mass Range (u): 45 to 500

Spectral Acquisition Rate: 20 spectra/second

Ion Source Temperature: 250°C

CHEMICAL IONIZATION at -140 eV

Reagent Gas: Methane

Acquired Mass Range (u): 45 to 500

Spectral Acquisition Rate: 20 spectra/second

Ion Source Temperature: 190°C

Instrument Control and Data Review:

ChromatOF optimized for TruTOF HT version 3.34

## 3. Results

Shown in Figure 1 are the chromatograms generated under EI conditions (a) and CI conditions (b). In each case, the chromatogram is plotted as  $m/z$  57 and alternating alkanes are labeled by carbon number.

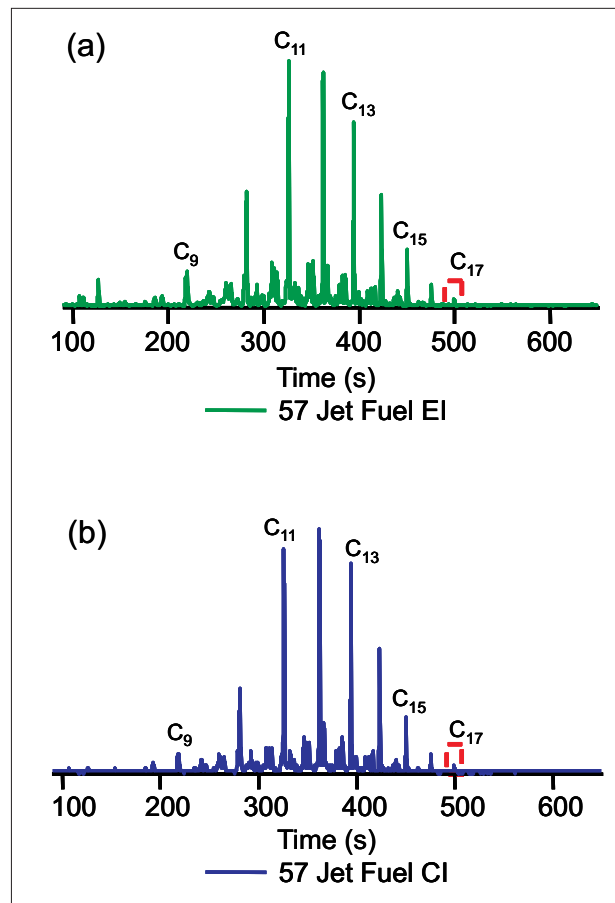


Figure 1. Chromatograms showing the separation of a Jet Fuel standard under (a) EI and (b) CI TOFMS conditions.

Note the similarity between the two chromatograms which is expected, since they were run under identical GC conditions. A diesel range organics standard was also injected under both EI and CI conditions in order to confirm the peak identifications. Mass spectra for  $n$ -C<sub>17</sub> (highlighted in red in Figure 1) are shown in Figure 2. For each spectrum shown in Figure 2, the molecular ion is highlighted in red. Spectrum (a) was generated under EI conditions and shows a very weak molecular ion signal at  $m/z$  240. This is to be expected according to the NIST spectrum which is shown in (b) and also has a very weak

molecular ion signal at  $m/z$  240. The fragmentation pattern observed on the TruTOF HT matches very well with the NIST spectrum and results in a library match score of 830 for Heptadecane ( $n\text{-C}_{17}$ ).

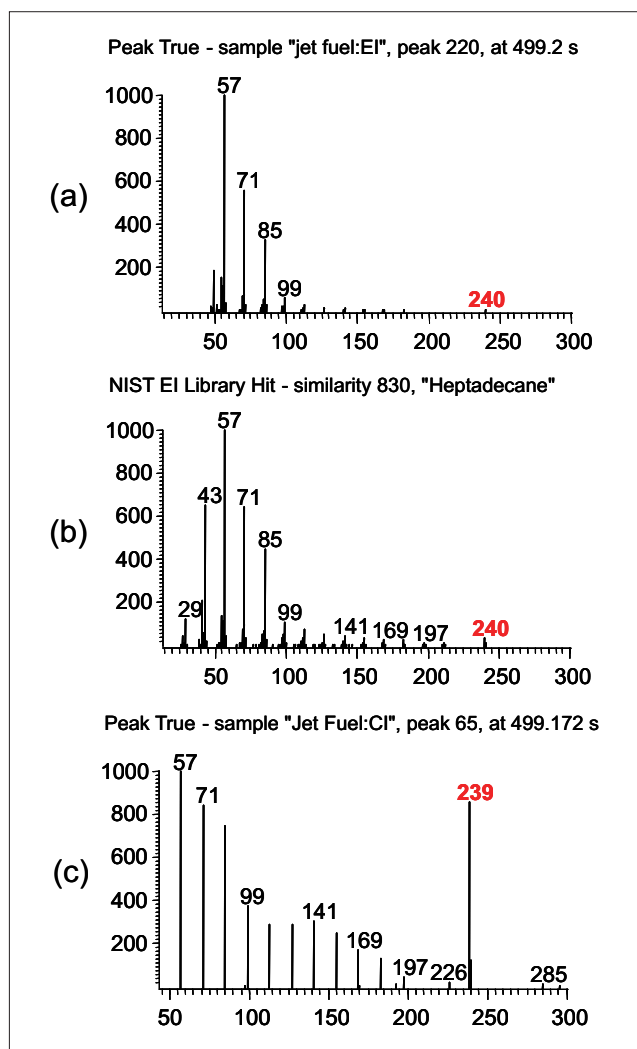


Figure 2. Mass spectra for the peaks highlighted in red in Figure 1. Shown are the (a) Peak True spectrum from the EI experiment, (b) NIST EI library hit for the EI experiment and (c) Peak True spectrum from the CI experiment.

The CI spectrum shown in Figure 2 (c) shows a very strong molecular ion signal at  $m/z$  239 (corresponding to the expected  $[M-H]^+$  signal). In this case, the CI spectrum also showed a significant amount of fragmentation further indicating the linear hydrocarbon structure.

#### 4. Conclusions

These experiments demonstrated the basic use of the TruTOF HT for the comparison of mass spectra generated in EI and CI mode. It is significant to note that these experiments were all performed on the same day and the system was changed from CI mode to EI mode in approximately 90 minutes. During this time the ion source chamber was vented, the ion sources were exchanged (from CI to EI), the ion source chamber was evacuated, the ion source was heated and finally the mass spectrometer was optimized. This fast changeover was made possible by the ion source gate valve which drastically reduces instrument downtime during routine TOFMS system maintenance.

