Application Snapshot

Instrument: LECO Pegasus BTX 4D

EMPOWERING RESULTS
Elemental Analysis | GC Mass Spectrometry | Metallography

Identifying Heteroatomic Species in HTL Pyrolysis Gasoline by GCxGC-TOFMS

LECO Corporation; Saint Joseph, Michigan USA

Key Words: Hydrothermal Liquefaction Pyrolysis Oil, GC-MS, GC-TOFMS, Deconvolution, Alternative Fuel, Sulfur

Hydrothermal liquefaction (HTL) is a high-pressure, moderate-temperature process used to produce biocrude oil and chemicals from biomass, providing more sustainable sources of fuel compared to traditional fossil fuels when wastes are used as feedstock. These complex products, which contain thousands of different individual components, require the enhanced chromatographic separation power of GCxGC for proper characterization. This is especially important for heteroatom-containing compounds known to have the potential to disrupt refining and treatment processes, leading to costly loss of catalysts or fouling of engines that could eventually use these fuels. Examples of trace-level analytes in a sample of gasoline-range pyrolysis oil formed from the HTL process are shown below, with filters applied to focus on the peaks that correspond to sulfur-, oxygen-, or nitrogen-containing compounds. GCxGC was crucial for separating the individual components in this complex sample and providing more accurate TOFMS identifications.

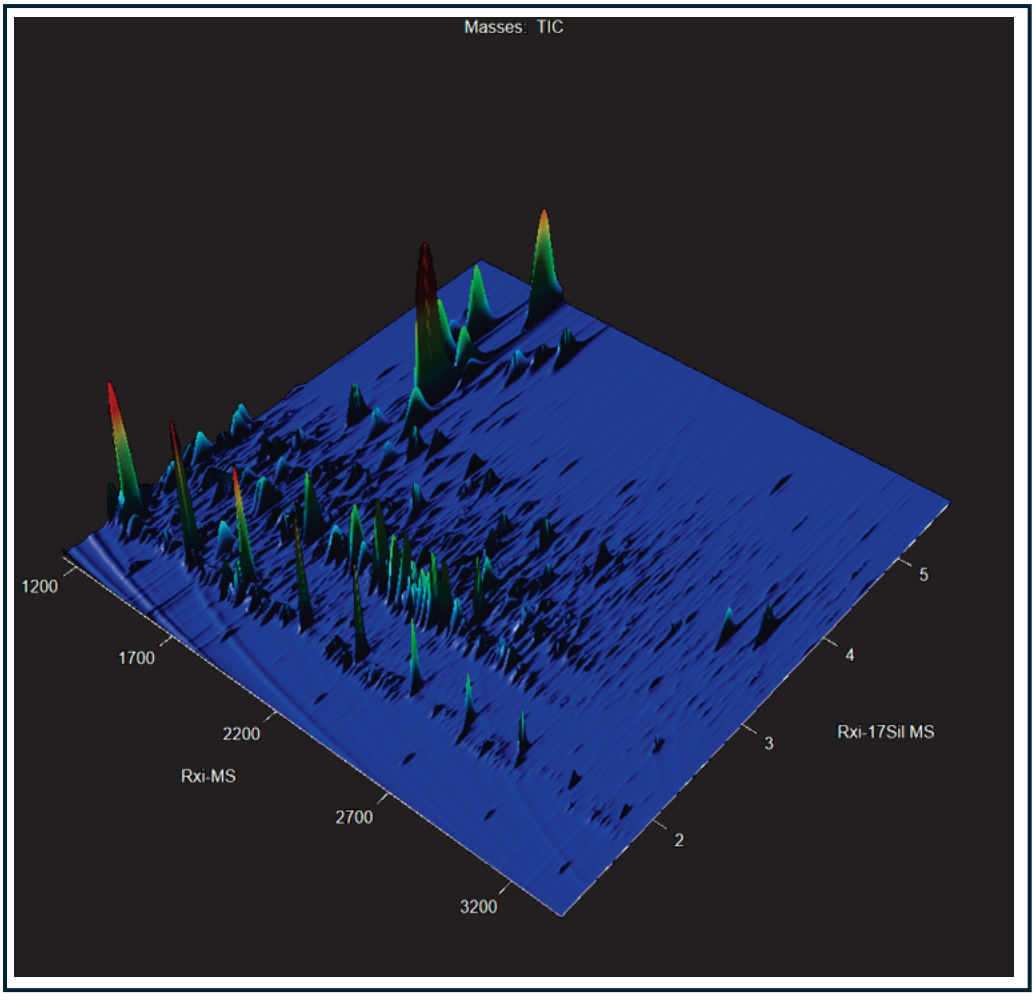

Figure 1. Surface plot showing total ion chromatogram (TIC) of heteroatom-rich region of HTL pyrolysis gasoline, demonstrating the complexity of the sample and enhanced chromatographic resolution of GCxGC.

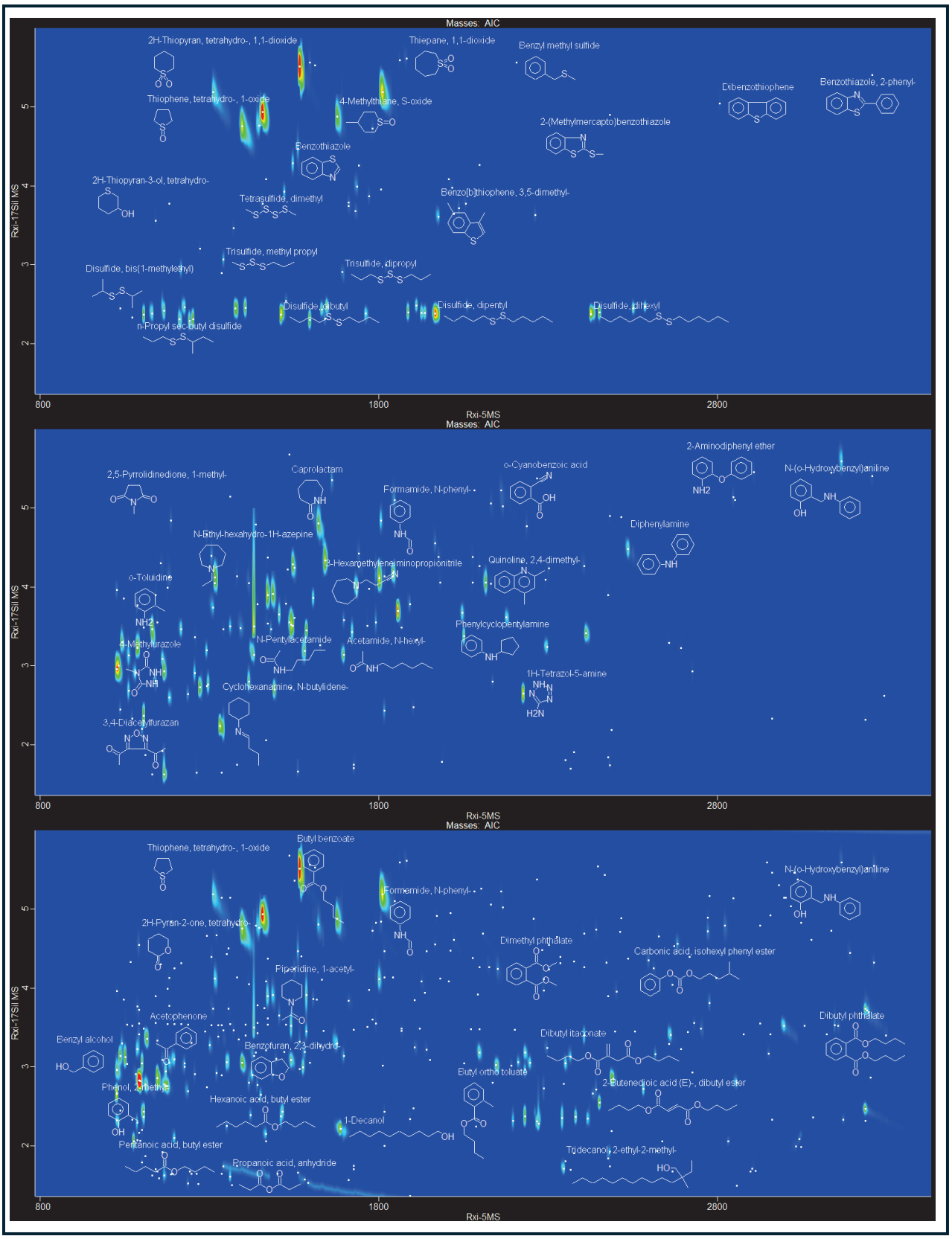

Figure 2. GCxGC contour plots showing filtered heteroatom-rich region of the chromatogram of HTL pyrolysis gasoline, plotting the analytical ion chromatogram (AIC) which displays only signal from peaks corresponding to each filter, requiring the presence of at least one sulfur (top), nitrogen (middle), or oxygen (bottom) heteroatom in the spectra-matched library formula. Note series of disulfides and trisulfides in the bottom of the left contour plot, demonstrating another advantage of GCxGC that aids with identification of peaks in a complex sample—elution bands of analytes based on structural similarities.