TECHNICAL BRIEF

ANALYSIS OF TOLUENE IN MIDDLE DISTILLATE OIL SAMPLES USING GAS CHROMATOGRAPHY AND THE LUMA™ MULTI-CHANNEL VACUUM ULTRAVIOLET (VUV) DETECTOR

VUV ANALYTICS

Introduction:

In the demanding field of petrochemical analysis, precision and reliability are paramount. Particularly when characterizing complex oil samples, it is essential to have a robust, sensitive, and highly selective method to ensure accurate results. One such critical analysis is the determination of toluene in oil samples. Toluene, a volatile aromatic compound, is often present in crude oils and refined petroleum products. Its concentration level can greatly influence the quality, safety, and usability of the oil, making its accurate detection crucial for the oil industry.

Traditional gas chromatography (GC) detectors may struggle with this task due to issues with co-elution, lack of selectivity, and sensitivity. Furthermore, they often require complex sample preparation, leading to extended analysis time and increased chances of error. This is where LUMA from VUV Analytics steps in to fill the gap.

LUMA, utilizing Vacuum Ultraviolet (VUV) spectroscopy, offers a solution that combines simplicity, sensitivity, and selectivity. Its wide range of detection (118 - 1050 nm) allows for a comprehensive examination of samples. In this technical brief, we demonstrate the utility of the LUMA detector in the analysis of toluene in oil samples. We show how the inherent benefits of the LUMA detector led to more accurate, efficient, and repeatable analysis, offering a practical solution to one of the petrochemical industry's fundamental challenges.

GC-LUMA Instrument Conditions for Toluene Analysis:

GC Conditions:	
Injection Volume: 1µL	**LUMA Conditions:**
Inlet Temperature: 250°C	**Makeup Gas Pressure:** 14 PSI N_2
Split Ratio: 10:1	**System Gas Pressure:** 52 psi N_2
Column: Rxi-1ms (30m x 0.25mm, 0.25µm)	**Flow Cell Temperature:** 275°C
Carrier gas: Hydrogen @ 2mL/min	**Transfer Line Temperature:** 275°C
Oven Program: 50°C, hold 0.1 min; 15°C/min to 270°C (15 min)	**Acquisition Rate:** 10 Hz
Run Time: 14 minutes	

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ISTD, QC Standard and Sample Preparation:

Internal Standard

To avoid interference in calculations, an ISTD of o-Xylene was prepared at [19.8 ppm] in dichloromethane.

QC Standards

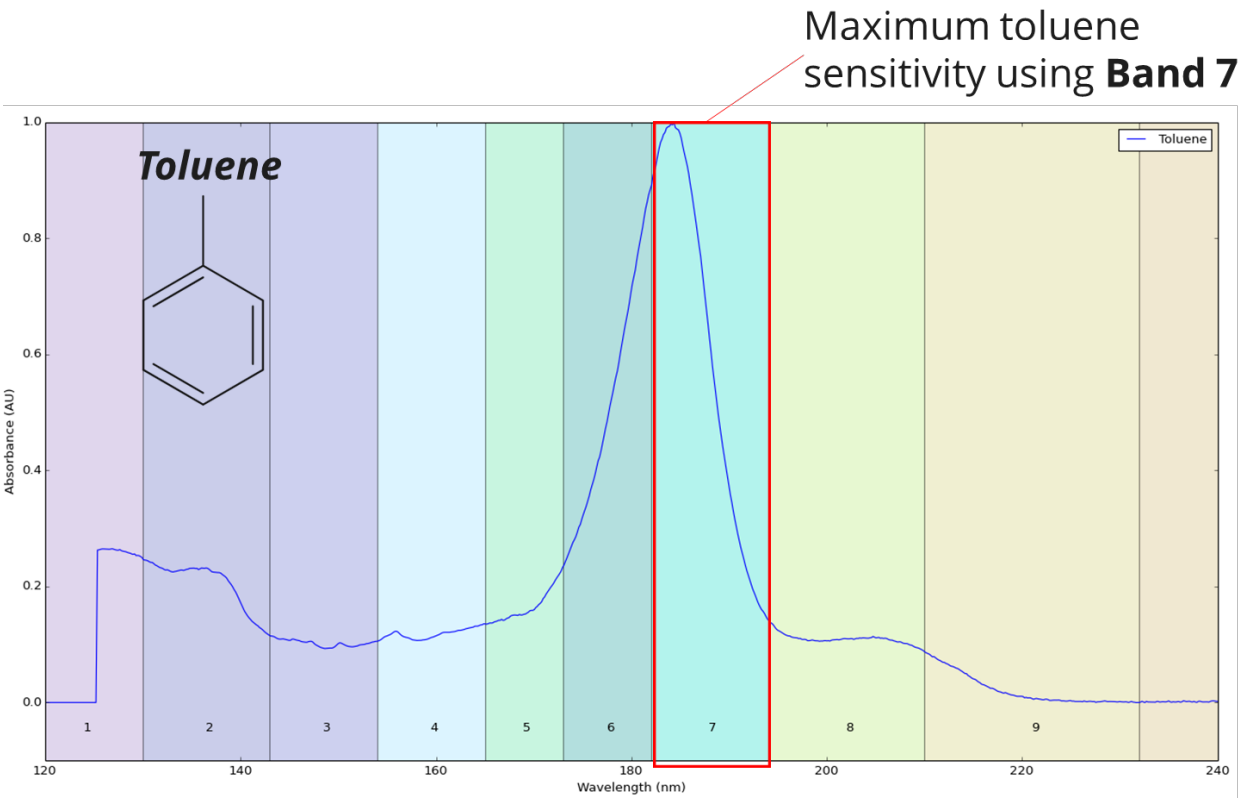
QC Toluene Standards were prepared at 10ppm and 30ppm.

Sample Preparation

50:50 dilution of sample oil + ISTD solution was used to get maximum amount on-column. The masses of sample oil and ISTD used were recorded for each sample mixture to calculate the amount of toluene found in the sample.

High Resolution VUV Spectra of Toluene:

For quantitation of analytes with LUMA the maximum absorbing band is used to obtain the best sensitivity and strongest analyte response. In this case, it's clear that Toluene has a maximum absorbance response in Band 7; hence, this Band will be used for its quantitation throughout the analysis.



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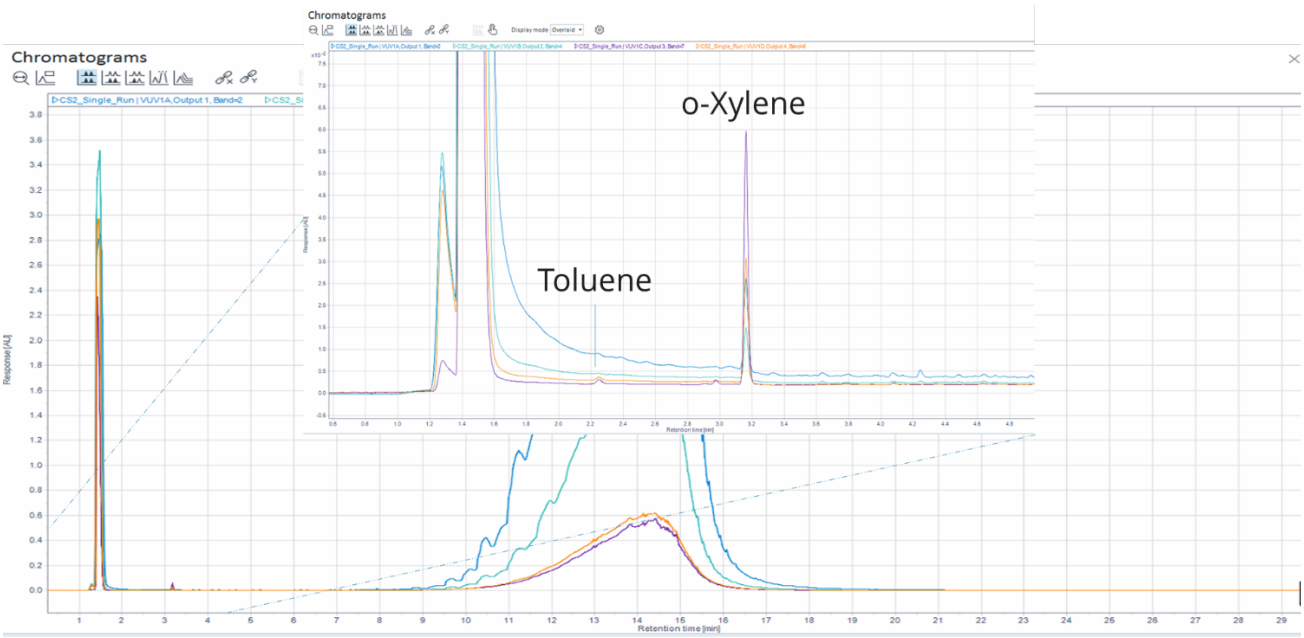
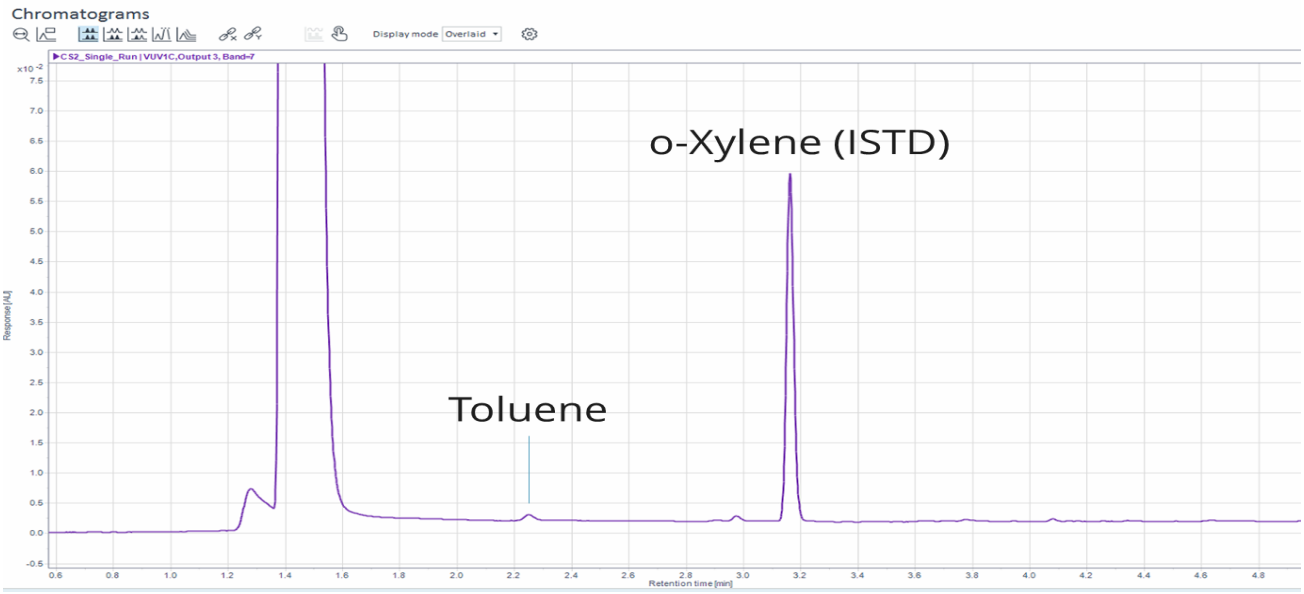
Results:

Middle Distillate Oil Sample # 1 Chromatogram (Bands 2, 4, 6 & 7 shown below)



Middle Distillate Oil Sample # 1 Chromatogram (Band7 shown below, used for quantitation)



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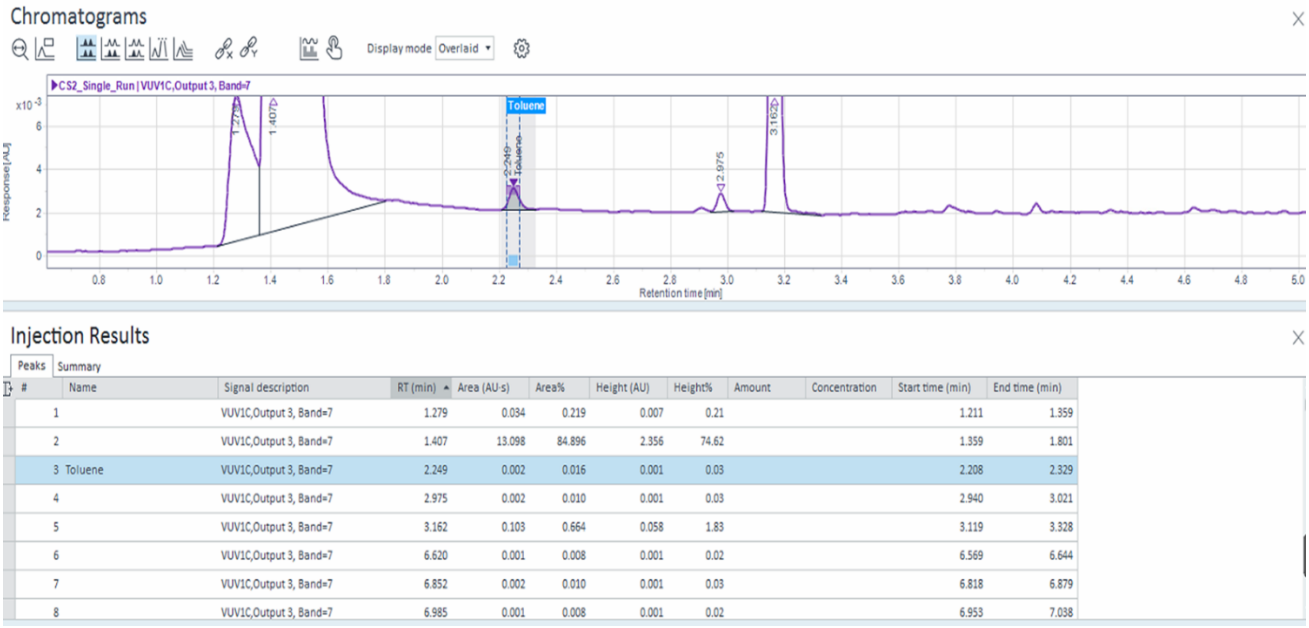
Middle Distillate Oil Sample # 1 Injection Results utilizing Band 7:



#	Name	Signal description	RT (min)	Area (AU·s)	Area%	Height (AU)	Height%	Amount	Concentration	Start time (min)	End time (min)
1		VUV1C,Output 3, Band=7	1.279	0.034	0.219	0.007	0.21			1.211	1.359
2		VUV1C,Output 3, Band=7	1.407	13.098	84.896	2.356	74.62			1.359	1.801
3	Toluene	VUV1C,Output 3, Band=7	2.249	0.002	0.016	0.001	0.03			2.208	2.329
4		VUV1C,Output 3, Band=7	2.975	0.002	0.010	0.001	0.03			2.940	3.021
5		VUV1C,Output 3, Band=7	3.162	0.103	0.664	0.058	1.83			3.119	3.328
6		VUV1C,Output 3, Band=7	6.620	0.001	0.008	0.001	0.02			6.569	6.644
7		VUV1C,Output 3, Band=7	6.852	0.002	0.010	0.001	0.03			6.818	6.879
8		VUV1C,Output 3, Band=7	6.985	0.001	0.008	0.001	0.02			6.953	7.038

*Toluene RT: 2.249 min, Area:0.002 AU*s, Height: 0.001 AU*

*o-Xylene RT: 3.162, Area:0.103 AU*s, Height: 0.058 AU*

The inherent OpenLab CDS features can be utilized to make Toluene results calculations following analysis with LUMA.

- **Calculate average response factor (F) using 10ppm and 30ppm QC samples**
- **Use F value to calculate remaining sample concentrations**

$$\frac{Peak\ Area_{Toluene}}{Concentration_{Toluene}} = F\frac{Peak\ Area_{o-Xylene}}{Concentration_{o-Xylene}} \Rightarrow Concentration_{Toluene} = \frac{Peak\ Area_{Toluene}\ x\ Concentration_{o-Xylene}}{Peak\ Area_{o-Xylene}\ x\ F}$$

Sample #	Predicted Toluene Concentration (ppm)	LUMA Calculated Toluene Concentration (ppm)
Sample 1	*(Blind)*	0.49
Sample 2	*(Blind)*	1.28
Sample 3	1.19	0.92
Sample 4	2.28	1.41
Sample 5	10.00	9.43
Sample 6	30.00	31.70

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Conclusion:

The application of LUMA for the determination of toluene in oil samples has showcased significant advantages in terms of sensitivity, selectivity, and simplicity over traditional GC methods. The data presented in this technical brief provides strong evidence of LUMA's high performance and efficiency in tackling one of the petrochemical industry's crucial challenges.

LUMA's wide detection range (118 - 1050 nm) empowers a comprehensive analysis of complex oil samples. It allows for an accurate determination of toluene, even at low concentrations, overcoming issues often encountered with traditional GC detectors, such as lack of sensitivity and co-elution problems.

Moreover, the use of LUMA simplifies the analytical workflow by reducing complex sample preparation, leading to reduced error probability and enhanced efficiency. The repeatable and reliable nature of the results assures analysts of the robustness and reliability of the method.

In summary, LUMA revolutionizes the analysis of toluene in oil samples, providing an innovative solution that balances simplicity, sensitivity, and selectivity. The ability to tackle the fundamental challenges in the petrochemical industry makes LUMA a valuable asset for petrochemical analysts and a significant step forward in oil characterization methods.