VGA-100 Instrument Detection Limits and Linearity

The VGA-100 is the world's first benchtop vacuum ultraviolet (VUV) spectrometer for gas chromatography (GC). It is a universal GC detector that provides both qualitative and quantitative data. The strong absorption of gas phase molecules in the VUV region of the ultraviolet spectrum (120 - 240 nm) provide excellent sensitivity, and the compound-specific absorption spectra provide unparalleled selectivity. VUV spectroscopy follows first principles detection and provides a predictable linear response that eliminates the need for continuous calibration. Analyte concentration can be easily determined by the Beer-Lambert Law used commonly in UV-VIS spectroscopy applications.



Demonstrated Instrument Performance

Quantitative analysis of compounds important to many industries including food & beverage, flavors & fragrances, petrochemical, and fuel refining was performed using the VGA-100 Gas Chromatography (GC) detector. Instrument detection limit (IDL) and linearity measurements of these compounds used a concentration range of 20 pg-50 ng. The VGA-100 IDLs averaged between 20-60 picograms (pg) on column with excellent linearity across three orders of magnitude.



Experimental Conditions

The following concentrations, sample replicates, GC settings, and data processing conditions were used unless otherwise noted. Instrument detection limit (IDL) and linearity measurements were taken across a concentration range of 20 pg-50 ng. Detection limits were calculated based upon a determination of the statistical variance in eleven replicate measurements at a low but detectable amount on column. A spectral filter of 140 - 160 nm was applied post-data acquisition to optimize for signal to noise.

VGA 100 Data acquisition rate: 4.5Hz

GC Oven: 70°C, hold 0.1 minutes; ramp at 20°C/min to 330°C, hold until last compound elutes

GC Injection volume: 1µl, 275°C Split injections, 4mm Precision split liner with wool

Paraffins

Paraffins are used in a variety of consumer products and separated in oil refineries by fractional distillation. This study measured n-Decane, n-Eicosane, n-Triacontane, and n-Tetracontane at concentrations between 50 pg-50 ng on column. Paraffin IDLs averaged 41 pg on column with an R^2 of 0.9945.

Experimental

A Restek certified reference material (Catalog # 31266) was used in the experiment. Detection limits were calculated based upon a determination of the statistical variance in ten replicate measurements at a low but detectable amount on column.

Paraffins							
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)		
n-Decane (C10)	1.8	40	50-50000	0.9990	140-160		
n-Eicosane (C20)	7.5	32	50-50000	0.9957	140-160		
n-Triacontane (C30)	11.4	35	50-50000	0.9872	140-160		
n-Tetracontane (C40)	14.6	55	50-50000	0.9960	140-160		

Figure 1: n-Decane, n-Eicosane, n-Triacontane, and n-Tetracontane IDL linearity data results from measurement with a VGA-100





Figure 2: n-Decane linearity plot showing VGA-100 measurement performance from 50 pg-50 ng on column

Polycyclic Aromatic Hydrocarbons

Polycyclic Aromatic Hydrocarbons (PAH) are ubiquitous, toxic compounds comprised of multiple aromatic rings. They commonly result from the incomplete combustion of organic matter and transformation of organic sediments into fossil fuels. This study measured Acenaphthylene, Fluorene, Benzo[a]pyrene, and Benzo[g,h,i]perylene at concentrations between 20 pg-20 ng and 20 pg-50 ng on column. PAH IDLs averaged 28 pg on column with an R² of 0.9936.

Experimental

A Restek certified reference material (Catalog # 31011) was used in the experiment. Detection limits were calculated based upon a determination of the statistical variance in twelve replicate measurements at a low but detectable amount on column. A spectral filter of 170 – 240 nm was applied post-data acquisition to optimize for signal to noise.

Polycyclic Aromatic Hydrocarbons						
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)	
Acenaphthylene	4.9	20	20-20000	0.9944	170-240	
Fluorene	5.4	33	20-50000	0.9988	170-240	
Benzo[a]pyrene	11.0	32	20-50000	0.9953	170-240	
Benzo[g,h,i]perylene	12.3	27	20-50000	0.9857	170-240	

Figure 3: Acenaphthylene, Fluorene, Benzo[a]pyrene, and Benzo[g,h,i]perylene IDL and linearity data results from measurement with a VGA-100





Figure 4: Fluorene linearity plot showing VGA-100 measurement performance from 20 pg-50 ng on column

Terpenes

Terpenes are commonly found in conifer plants and are key ingredients in flavor, fragrance, and alternative medicine applications. This experiment measured alpha-Pinene, gamma-Terpinene, Geraniol, and alpha-Bisabolol. Terpene IDLs averaged 28 pg on column with an R² of 0.9971.

Experimental

A Restek certified reference material (Catalog # 34095) was used in the experiment.

GC Oven: 40°C, hold 0.1 minutes; ramp at 15°C/min to 250°C, hold until last compound elutes

Terpenes						
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)	
α-Pinene	3.3	25	20-50000	0.9982	140-160	
gamma-Terpinene	4.5	15	20-50000	0.9972	140-160	
Geraniol	6.4	25	20-50000	0.9972	140-160	
α-Bisabolol	9.9	45	20-50000	0.9957	140-160	

Figure 5: alpha-Pinene, gamma-Terpinene, Geraniol, and alpha-Bisabolol linearity data results from measurement with a VGA-100





Figure 6: alpha-Pinene linearity plot showing VGA-100 measurement performance from 20 pg-50 ng on column

FAMEs

Fatty acids and their corresponding methyl esters (FAMEs) are important analytes for consideration in terms of food science, nutrition, and bio-based fuels. This experiment measured Methyl Decanoate, Methyl Laurate, Geraniol, Methyl Palmitate, and Methyl Docosanoate at concentrations between 20 pg-50 ng and 50 pg-50 ng on column. FAME IDLs averaged 34 pg on column with an R² of 0.9940.

Experimental

A Sigma Aldrich certified reference material (Catalog # 49453-U) was used in the experiment.

FAMES							
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)		
Methyl Decanoate	3.8	30	20-50000	0.9963	140-160		
Methyl Laurate	5.0	25	50-50000	0.9947	140-160		
Methyl Palmitate	7.2	35	20-50000	0.9920	140-160		
Methyl Docosanoate	9.8	45	50-50000	0.9931	140-160		

GC Oven: 70°C, hold 0.1 minutes; ramp at 20°C/min to 300°C, hold until last compound elutes

Figure 7: Methyl Decanoate, Methyl Laurate, Methyl Palmitate, and Methyl Docosanoate linearity data results from measurement with a VGA-100





Figure 8: Methyl Decanoate linearity plot showing VGA-100 measurement performance from 20 pg-50 ng on column

Fragrance Allergens

Cosmetic products are typically required to label fragrance compounds having concentrations exceeding 100 ppm. This study measured standard mixtures Fragrance Allergen [A], [B], and [C] from Restek at concentrations between 20 pg-20 ng on column. Fragrance allergen [A], [B], and [C] IDLs averaged 35, 44, and 36 pg on column with R² of 0.9938, 0.9952, 0.9910, respectively.

Fragrance Allergen [A] Experimental

A Restek certified reference material (Catalog # 33102) was used in the experiment.

Fragrance Allergens (STD A)							
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)		
Phenylacetaldehyde	2.1	40	20-20000	0.9960	140-160		
Lilial	5.1	30	20-20000	0.9923	140-160		
α-Amylcinnamaldehyde	5.8	35	20-20000	0.9957	140-160		
α-Hexylcinnamaldehyde	6.3	35	20-20000	0.9912	140-160		

Figure 9: Phenylacetaldehyde, Lilial, alpha-Amylcinnamaldehyde, and alpha-Hexylcinnamaldehyde linearity data results from measurement with VGA-100





Figure 10: Phenylacetaldehyde linearity plot showing VGA-100 measurement performance from 20 pg-20 ng on column

Fragrance Allergen [B] Experimental

A Restek certified reference material (Catalog # 33103) was used in the experiment.

Fragrance Allergens (STD B)						
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)	
Citronellol	3.2	65	20-20000	0.9953	140-160	
Geraniol	3.4	35	20-20000	0.9951	140-160	
Eugenol	4.0	35	20-20000	0.9947	140-160	
Methyl Eugenol	4.3	40	20-20000	0.9955	140-160	

Figure 11: Citronellol, Geraniol, Eugenol, and Methyl Eugenol linearity data results from measurement with VGA-100



Figure 12: Citronellol linearity plot showing VGA-100 measurement performance from 20 pg-20 ng on column



Fragrance Allergen [C] Experimental

Fragrance Allergens (STD C)							
Analyte	Retention Time (Minutes)	IDL (pg)	Linear Dynamic Range (pg)	R ²	λ Integration Range (nm)		
Camphor	2.7	30	20-20000	0.9923	140-160		
Coumarin	4.5	35	20-20000	0.9936	140-160		
lso-a-Methylionone	4.8	30	20-20000	0.9906	140-160		
Benzyl Cinnamate	8.0	50	20-20000	0.9874	140-160		

A Restek certified reference material (Catalog # 33104) was used in the experiment.

Figure 13: Camphor, Coumarin, Iso-alpha-Methylionone, and Benzyl Cinnamate linearity data results from measurement with VGA-100



Figure 14: Coumarin linearity plot showing VGA-100 measurement performance from 20 pg-20 ng on column



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