Fast Analysis of Non-Traditional Gasoline Additives with Gas Chromatography-Vacuum Ultraviolet Spectroscopy

Ryan Schonert, Dan Wispinski, Jack Cochran

VUV ANALYTICS


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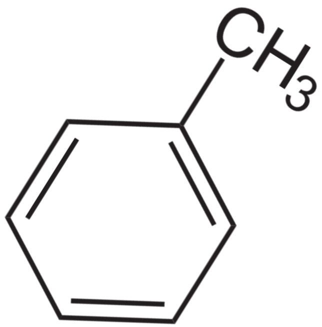
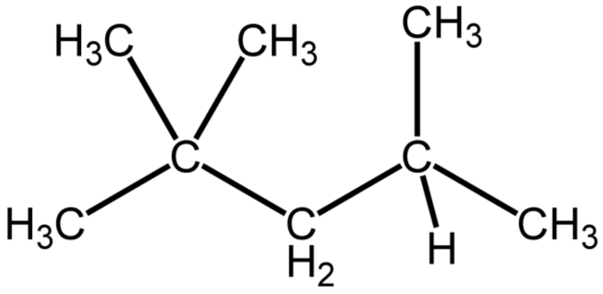
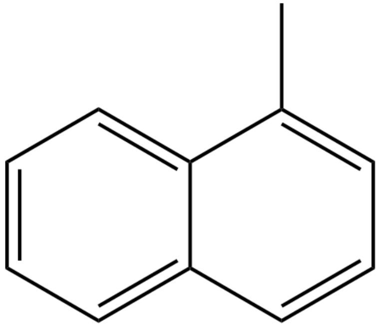
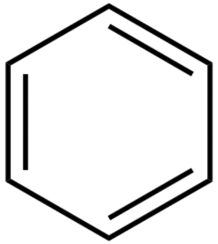
Gasoline Additives

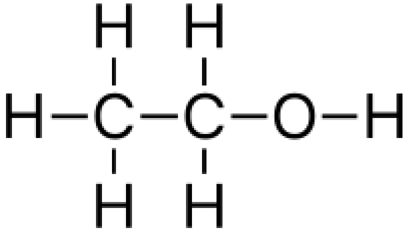
- Organic compounds which adjust fuel properties
  - Refining process, store-bought
- Major fuel blending components: octane boosters, pollution preventers
  - Blended at volume % level

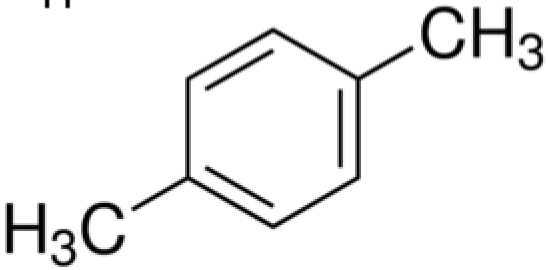


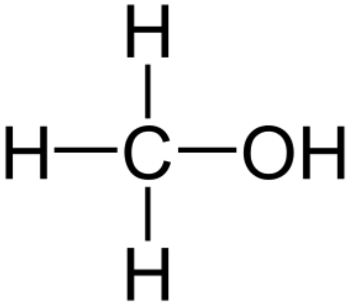












Groysman, A. (2014). Corrosion in Systems for Storage and Transportation of Petroleum Products and Biofuels Identification, Monitoring and Solutions. Ch. 2: Fuel Additives. Springer Science+Business Media Dordrecht.

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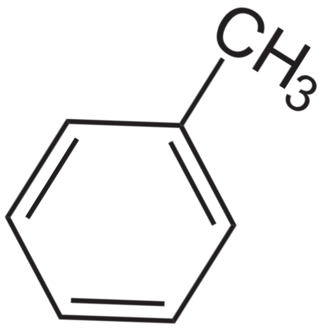

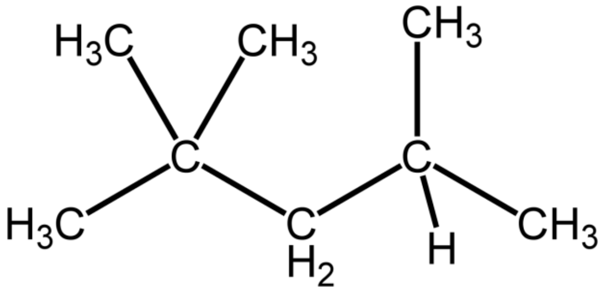

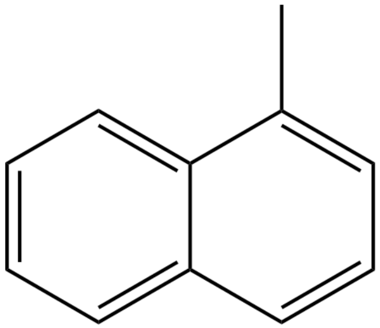

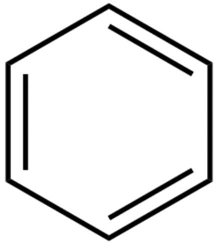

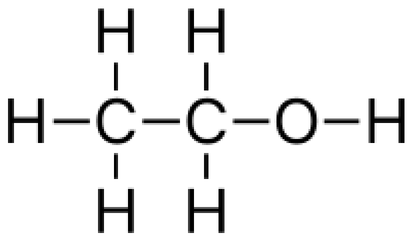

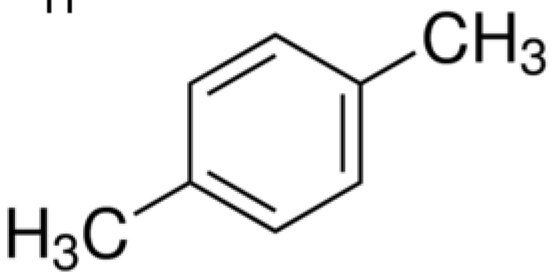

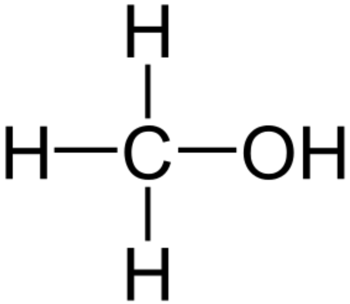

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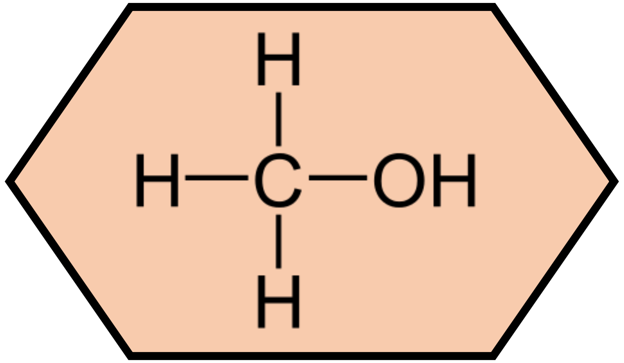
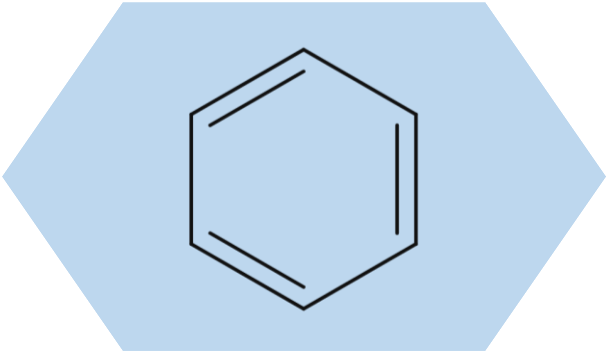
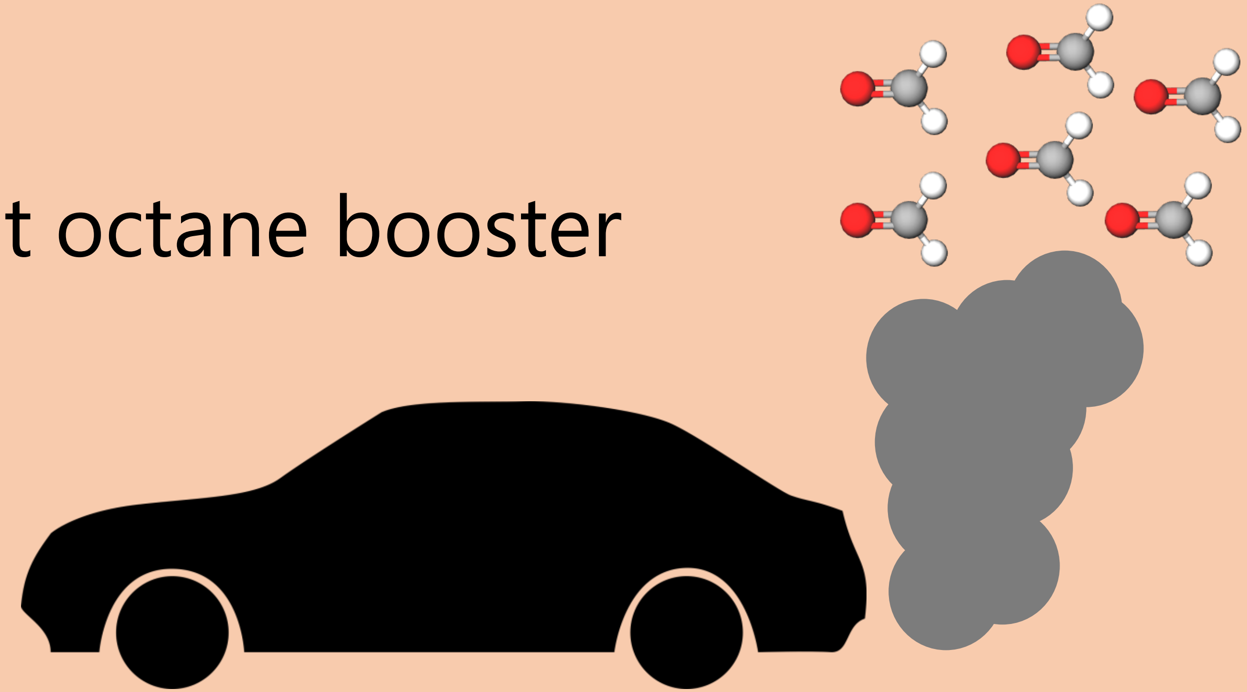


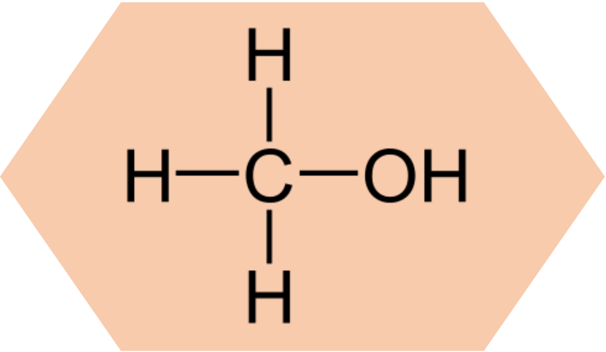


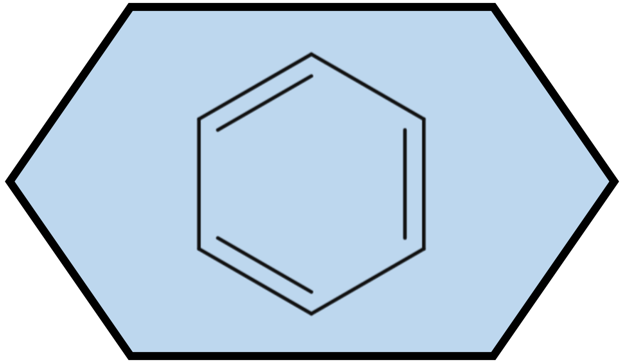
Methanol

- Cheap and efficient octane booster
- Emissions: high formaldehyde concentrations



Methanol Institute (n.d.). Methanol Use in Gasoline. Methanol Institute. Web.





Benzene

- Important BTEX octane-boosting component
- Group 1 carcinogen

Trojan UV (2010). Update on Emerging Contaminants: Fuel and Fuel Additives. Trojan UV / Trojan Technologies. Web.

Non-Traditional Gasoline Additives (NTGAs)

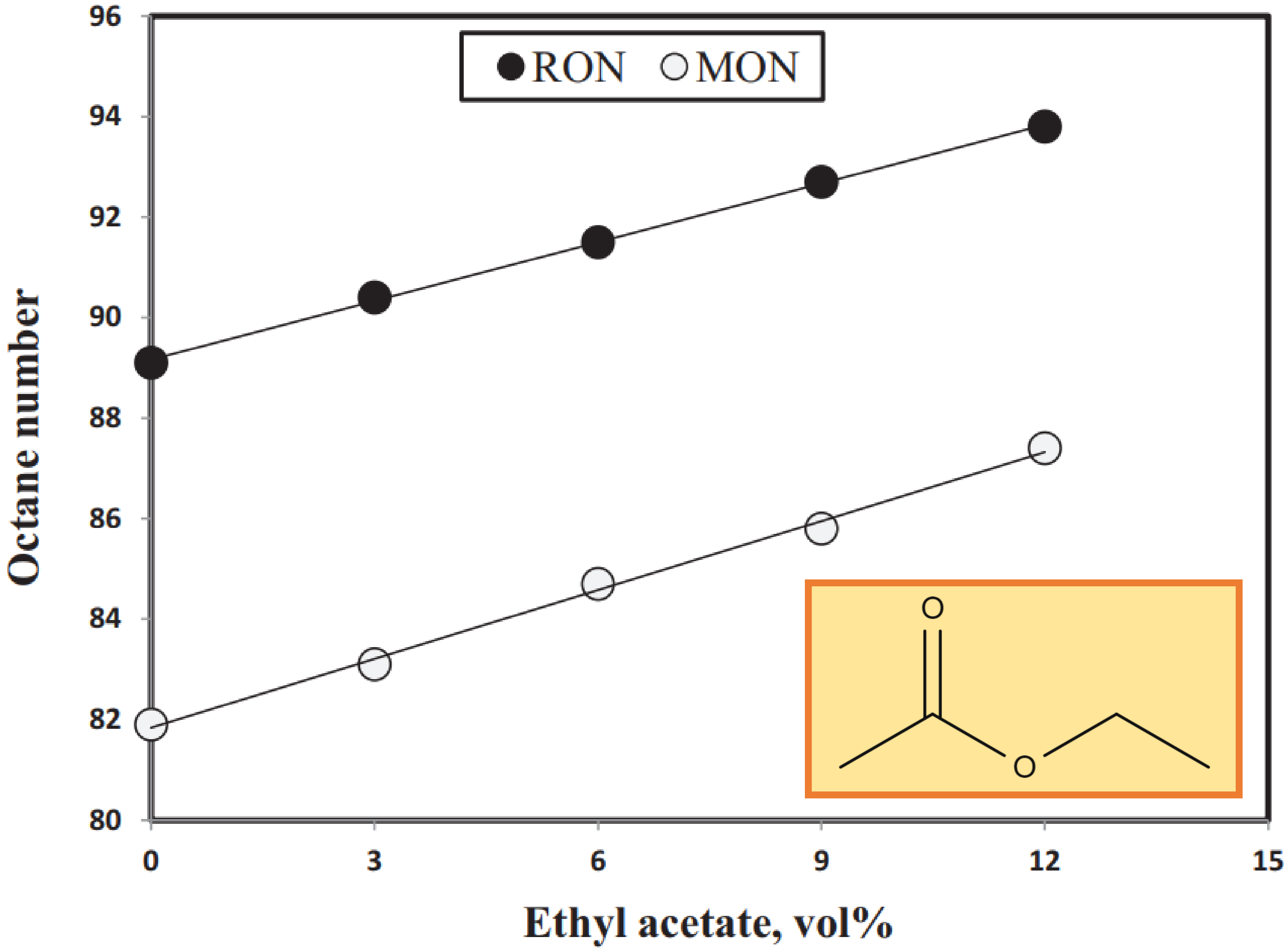
Desired Effect

+

Environmentally Safe

+

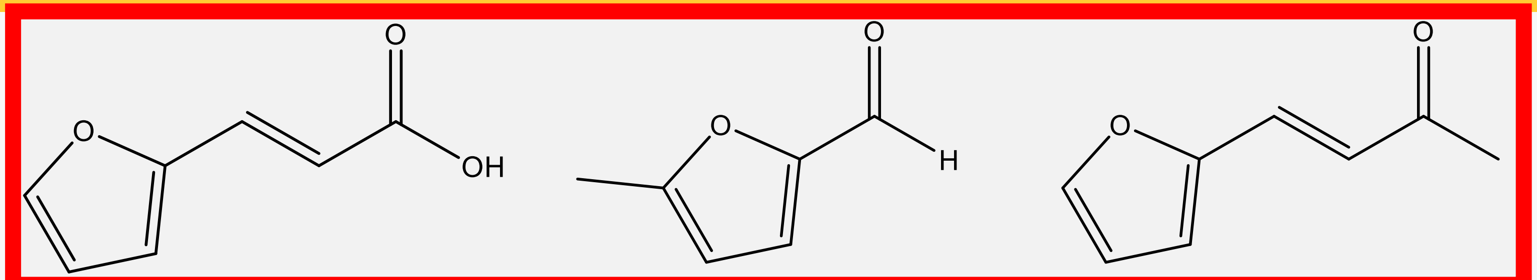
Renewable



Amine, M. et al. (2017). Effect of Ethyl Acetate Addition on Phase Stability, Octane Number, and Volatility Criteria of Ethanol-Gasoline Blends. Egyptian Journal of Petroleum, https://doi.org/10.1016/j.ejpe.2017.08.007.

Cuadernos de Investigación UNED

UNED Research Journal



Pineapple-stover derived furan compounds as gasoline oxygenate additive

Andrea P. Irías-Mata, Giselle Lutz

Abstract

Furan compounds have properties such as oxygenate additive to enhance octane number of gasoline. The procedure was a furan synthesis through an acidic hydrolysis of the polysaccharide materials from pineapple plantation residues. The products obtained were a complex mixture of mostly 3-(2-furanyl)-2-propenoic acid, 4-(2-furanyl)-3-butene-2-one and 5-methyl-furfural. Thermodynamic and rheolgical properties of the mixture *in toto* were measured, as well as its oxygenating capability. The results showed a two units enhancer oxygenate additive for naphta, potentially safe for transport and handling, presenting the following characteristics: specific gravity 1,22559±0,00002, kinematic viscosity 0,0127±0,0001 Stokes, enthalpy of vaporization 39,1±0,1kJ mol^{-1}, isothermal compressibility (1,0±0.2)$10^{-9}Pa^{-1}$, rate of evaporation 0,03±0,02g s^{-1} m^{-2} and Hildebrand solubility parameter 18,0±0,1$(J\ cm^{-3})^{1/2}$.

KEY WORDS

Pineapple crown, pineapple stubble, research octane number, oxygenate additive, furan compound, methyl terbutyl ether.

2017-01-0868

Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines

Robert L. McCormick, Gina Fioroni, Lisa Fouts, and Earl Christensen
National Renewable Energy Laboratory

Janet Yanowitz
Ecoengineering Inc.

Evgueni Polikarpov, Karl Albrecht, and Daniel J. Gaspar
Pacific Northwest National Laboratory

John Gladden and Anthe George
Sandia National Laboratory

Biomass-derived compounds that have potential as fuel blendstocks (partial list)

Name	Formula	CAS#	RON (D2699)	MON (D2700)	HOV, kJ/kg [a]	LHV, MJ/kg	LHV, MJ/L (at 20°C)	Density, g/L (at 20°C)	Water Solubility, mg/L
Alcohols									
Methanol	CH_4O	67-56-1	109	89	1173.5	20.09	15.8	786.4	miscible
Ethanol	C_2H_6O	64-17-5	109	90	918.2	25.54	20.2	789.3	miscible
n-Propanol [c]	C_3H_8O	71-23-8	104	89	788.7	30.8	24.7	811.0	miscible
2-propanol [c]	C_3H_8O	67-63-0	109	97	743.8	30.7	24.1	781.2	miscible
1-Butanol	$C_4H_{10}O$	71-36-3	98	85	708.3	33.1	26.8	805.7	68,000
2-butanol	$C_4H_{10}O$	78-92-2	107	93	670.5	33.1	26.7	802.6	181,000
2-methylpropan-1-ol (isobutanol)	$C_4H_{10}O$	78-83-1	105	90	685.4	33.2	26.6	797.6	85,000
2-methyl-1-butanol	$C_5H_{12}O$	137-32-6	101	88.3	613.7	34.69	28.3	814.8	29,700
2-pentanol	$C_5H_{12}O$	6032-29-7	99.4	90.8	608.1	34.58	27.8	805.2	44,600
Alkanes									
Triptane (2,2,3-trimethylbutane) [c]	C_7H_{16}	464-06-2	112	101	319.3	44.4	30.8	694.5	29
Alkenes									
Diisobutylene (a mixture of three parts 2,4,4-trimethyl-1-pentene and one part 2,4,4-trimethyl-2-pentene)	C_8H_{16}	25167-70-8	106	86.5	318.2	44.27	31.66	715.1	4
Esters									
Methylacetate	$C_3H_6O_2$	79-20-9	>120	>120	438.7	19.3	17.9	927.1	243,000
Methylbutanoate [c]	$C_5H_{10}O_2$	623-42-7	107.2	105	401.4	26.07	23.25	892.2	15,000
Methylisobutanoate (2-methylpropanate) [c]	$C_5H_{10}O_2$	547-63-7	103.6	104.7	365.2	28.38	25.04	882.4	9,260
Methylpentanoate [c]	$C_6H_{12}O_2$	624-24-8	103.4	101.1	379.6	28.25	24.99	884.8	2,200
Methyl-2-methylbutanoate [c]	$C_6H_{12}O_2$	868-57-5	110.5	99.1	338.3 [b]	28.08	24.59	875.7	3,200
Ethylacetate	$C_4H_8O_2$	141-78-6	118	>120	399.5	23.79	21.34	894.6	80,000
Ethylbutanoate	$C_6H_{12}O_2$	105-54-4	115.4	106	369.3	28.64	25.17	874.3	4,900
Ethylisobutyrate (2-methylpropanoate) [c]	$C_6H_{12}O_2$	97-62-1	110.3	109.5	342.6	30.44	26.46	869.3	3,200
1-Methylethylacetate (isopropylacetate) [c]	$C_5H_{10}O_2$	108-21-4	>120	--	363.3	25.77	22.47	871.8	29,000
Butylacetate	$C_6H_{12}O_2$	123-86-4	100.8	100	369.3	27.43	24.03	876.0	8,400
Isobutylacetate (2-methylpropylacetate) [c]	$C_6H_{12}O_2$	110-19-0	108.7	112.3	319.4	28.01	24.4	871.2	6,300
Isoamylacetate (3-methylbutylacetate) [c]	$C_7H_{14}O_2$	123-92-2	100.6	97.2	356.4	32.15	27.84	866.1	2,000
Ethers									
Methoxybenzene (anisole)	C_7H_8O	100-66-3	103	92	428.2	33.5	33.3	989.2	1,040
Furans									
2-Methylfuran/2,5-dimethylfuran mixture (40/60 by weight)	--	--	102	87		32.2	29.1	903	2,240
Ketones									
2-Butanone (methyl ethyl ketone)	C_4H_8O	78-93-3	111	105.5	481.2	31.36	25.08	799.8	223,000
2-Pentanone	$C_5H_{10}O$	107-87-9	105.7	103	445.8	33.37	26.75	801.5	43,000
3-Pentanone [c]	$C_5H_{10}O$	96-22-0	106.8	--	448.2	33.43	27.08	810.1	45,900
3-Methyl-2-butanone [c]		563-80-4	108.9	102.2	428.4	33.34	26.68	815.0	5,237
Cyclopentanone	C_5H_8O	120-92-3	101	89.4	504.0	31.99	30.2	944.1	60,000
3-Hexanone [c]	$C_6H_{12}O$	589-38-8	101.9	93.5	417.3	34.83	28.61	821.6	14,700
4-Methyl-2-pentanone (methylisobutyl ketone) [c]	$C_6H_{12}O$	108-10-1	105.7	105.5	417.3	34.21	27.27	797.1	19,000
2,4-dimethyl-3-pentanone	$C_7H_{14}O$	565-80-0	99	92.5	363.4	35.84	28.81	803.9	5,700
Ketone mixture (42.5 wt% 2-pentanone, 11.4 wt% methyl-isobutyl ketone, 30.3 wt% 4-heptanone, 15.8 wt% 2-heptanone)	--	--	99.4	99.6	424 [b]	34.61	27.99	808.7	--

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Harmful NTGAs

Methyl Acetate	Acetone
N-Methylaniline	Methylal
Secondary-Butyl Acetate	

"Considered to be a cheap source of octane, these chemicals could cause engine problems…[t]hey are also harmful to human health and to the environment…"

ACFA (2014). Report on Harmful Chemicals in Gasoline Blending. ACFA. Web.

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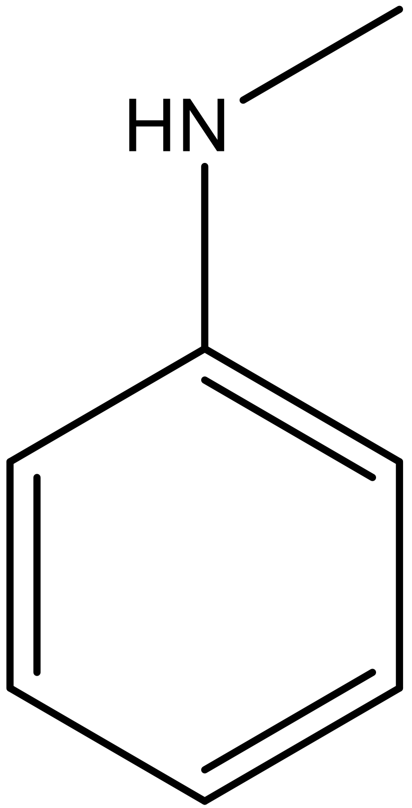


- **Octane booster**
- **Causes gum formation** – carbon deposit in engine parts
- **Swells rubber seals** – may cause oil leaks

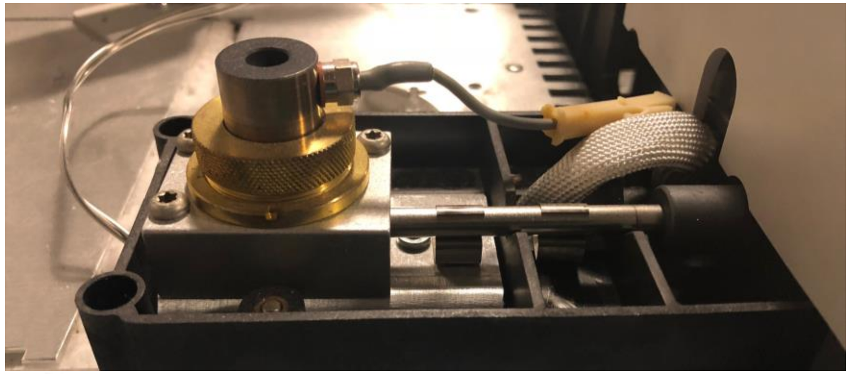
ACFA (2014). Report on Harmful Chemicals in Gasoline Blending. ACFA. Web.

Gasoline Analysis – DHA, ASTM D6730

- *2+ hour run time*
- *Identification by retention time only*
- ***Not equipped to analyze novel compounds***

INTERNATIONAL

Designation: D6730 – 01 (Reapproved 2016)



Standard Test Method for Determination of Individual Components in Spark Ignition Engine Fuels by 100–Metre Capillary (with Precolumn) High-Resolution Gas Chromatography[1]

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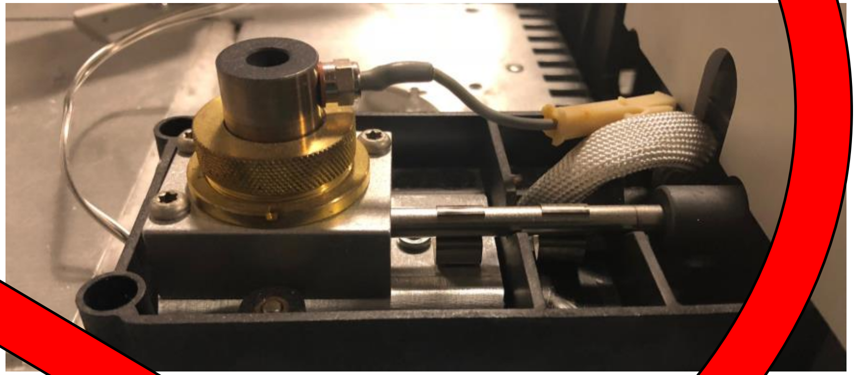
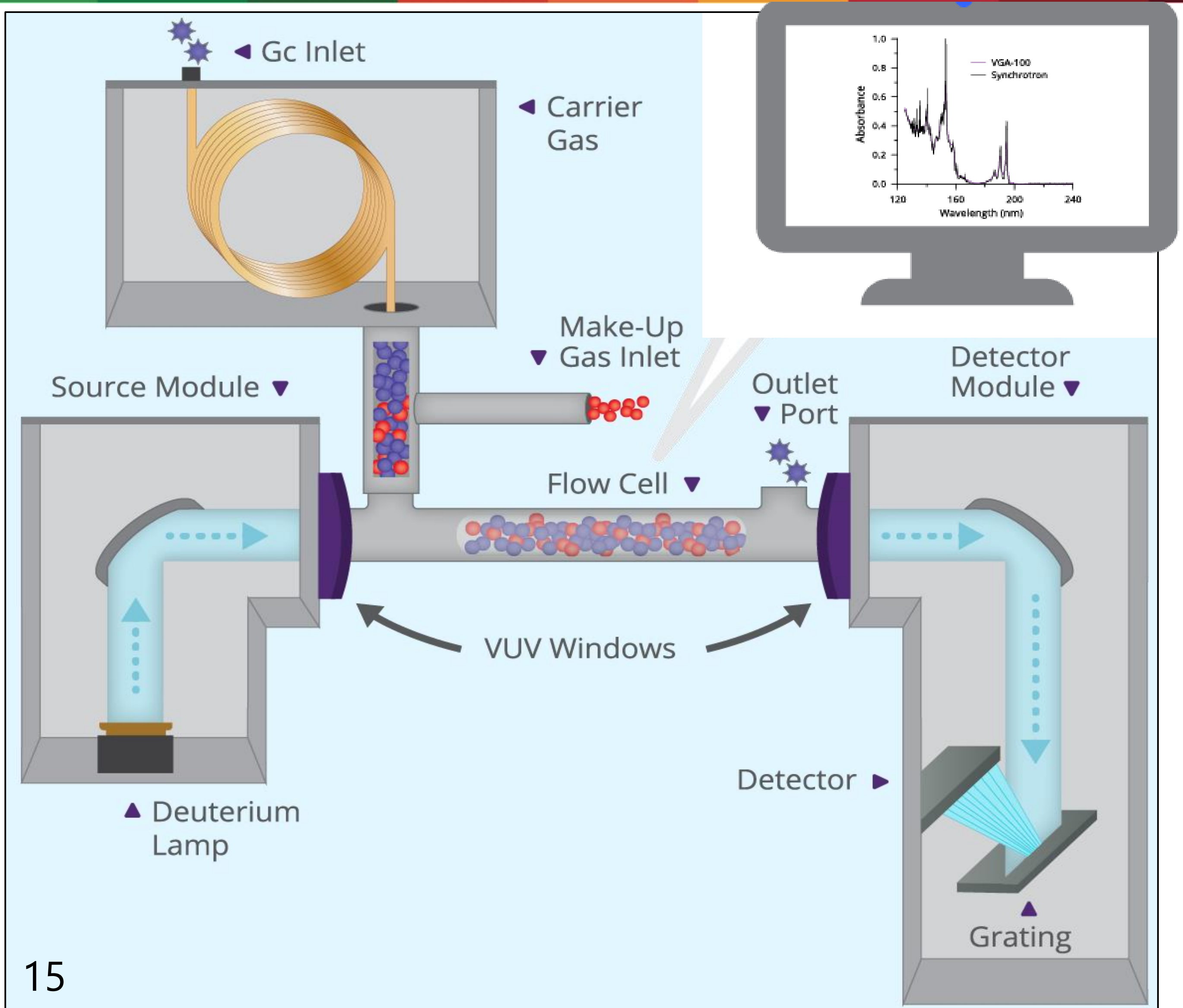
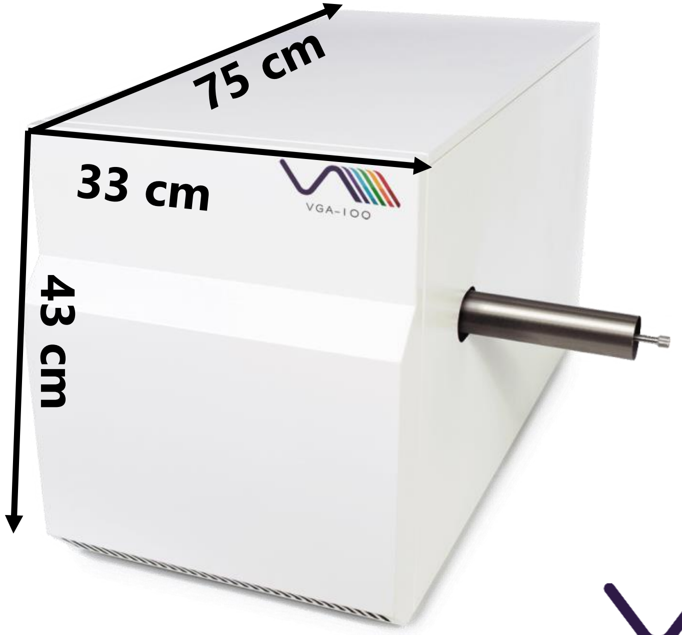


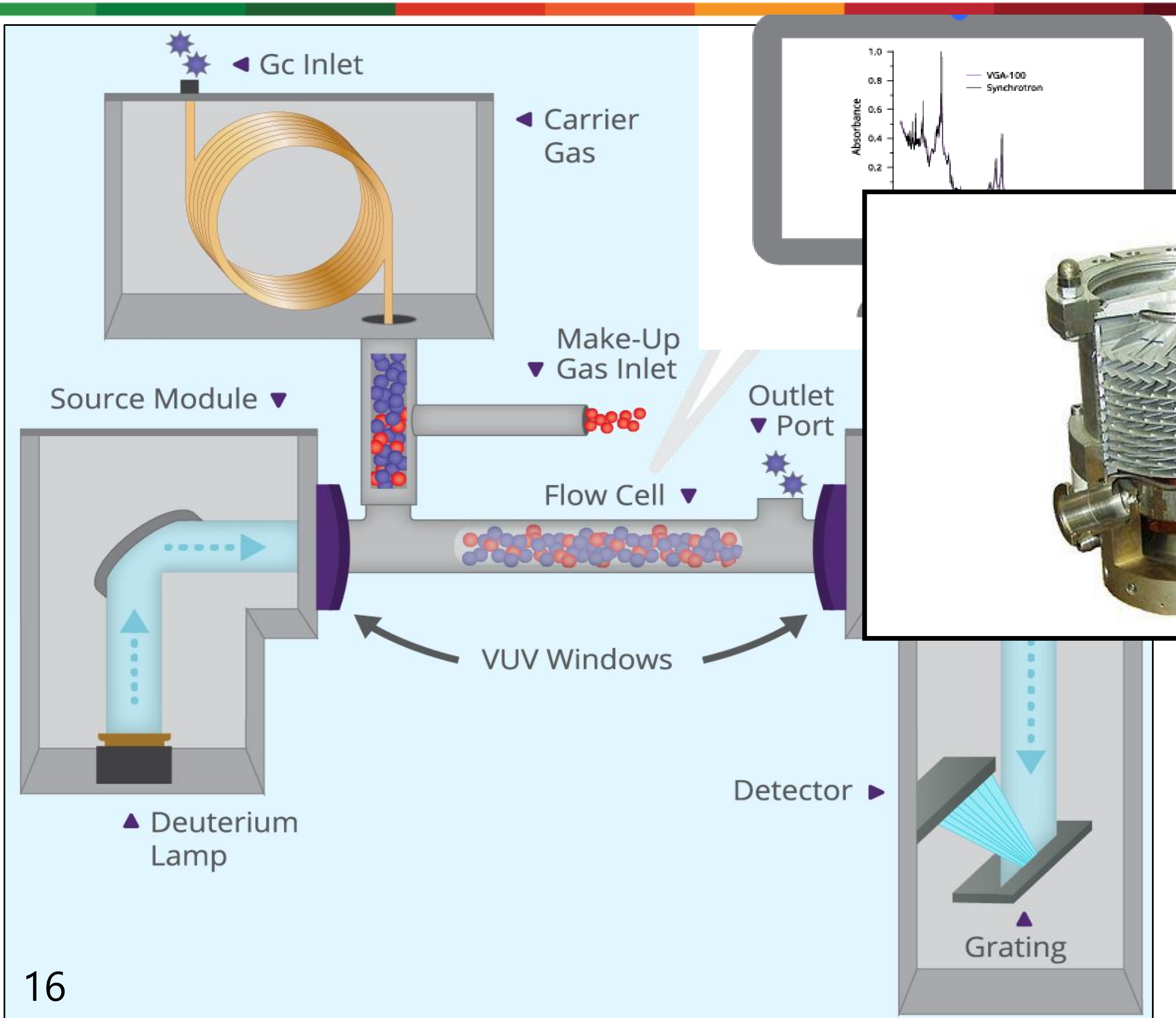
How Does VUV Spectroscopy Work?



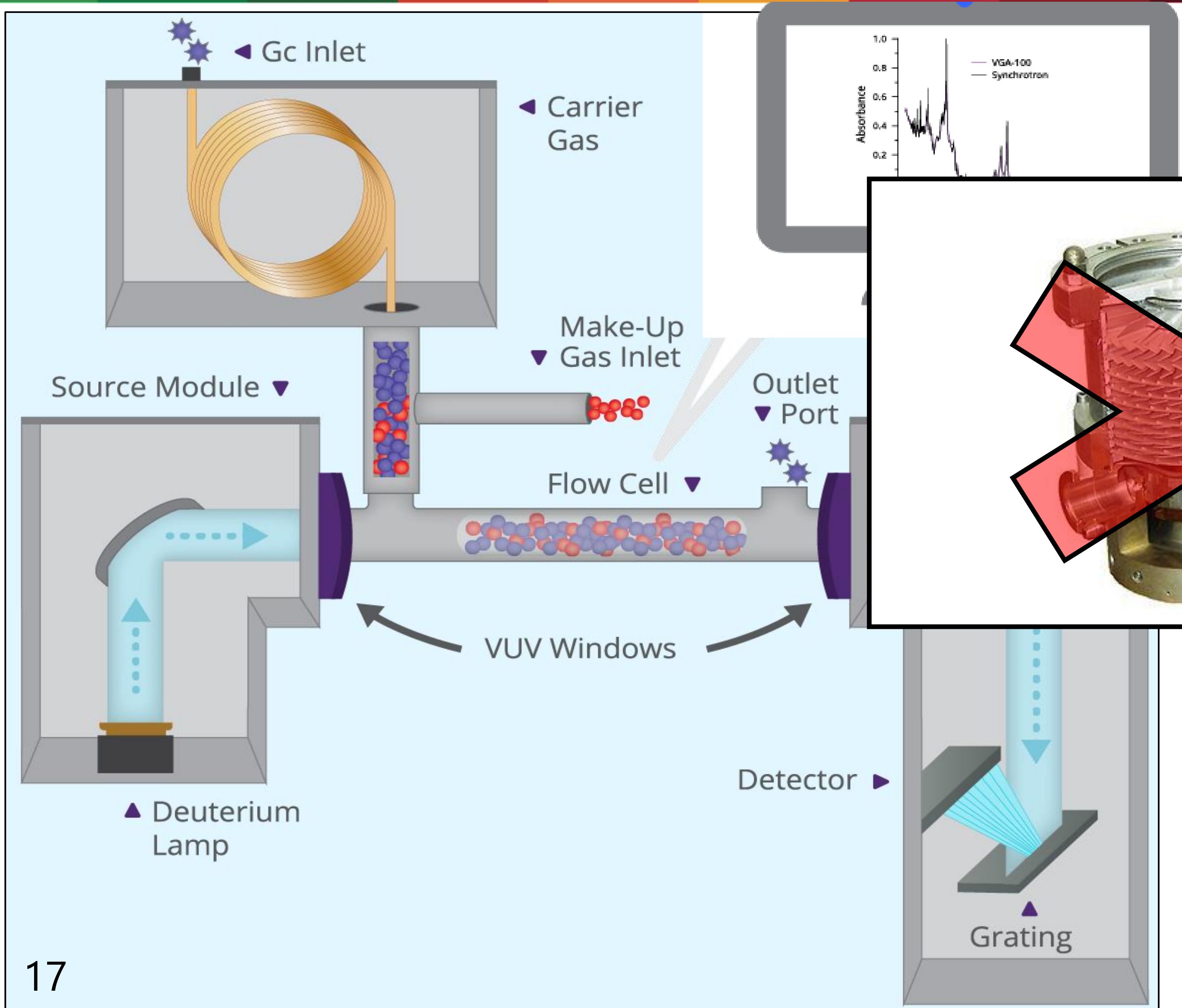
VUV Analytics VGA-100
125 to 240nm
1 to 75 spectra/sec

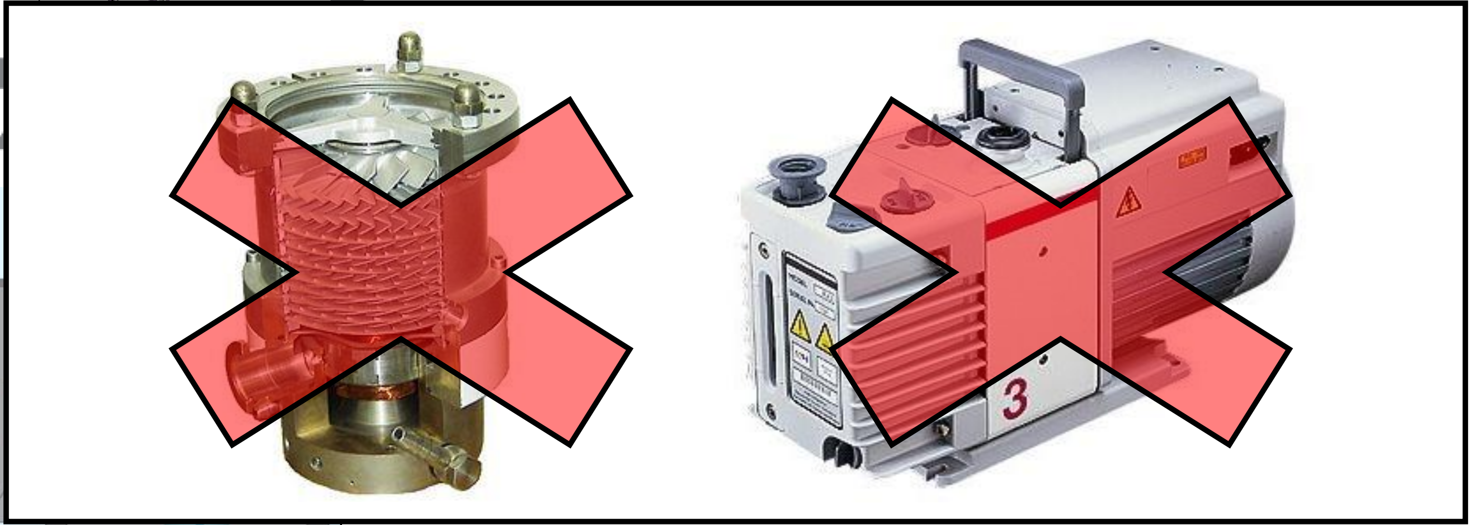


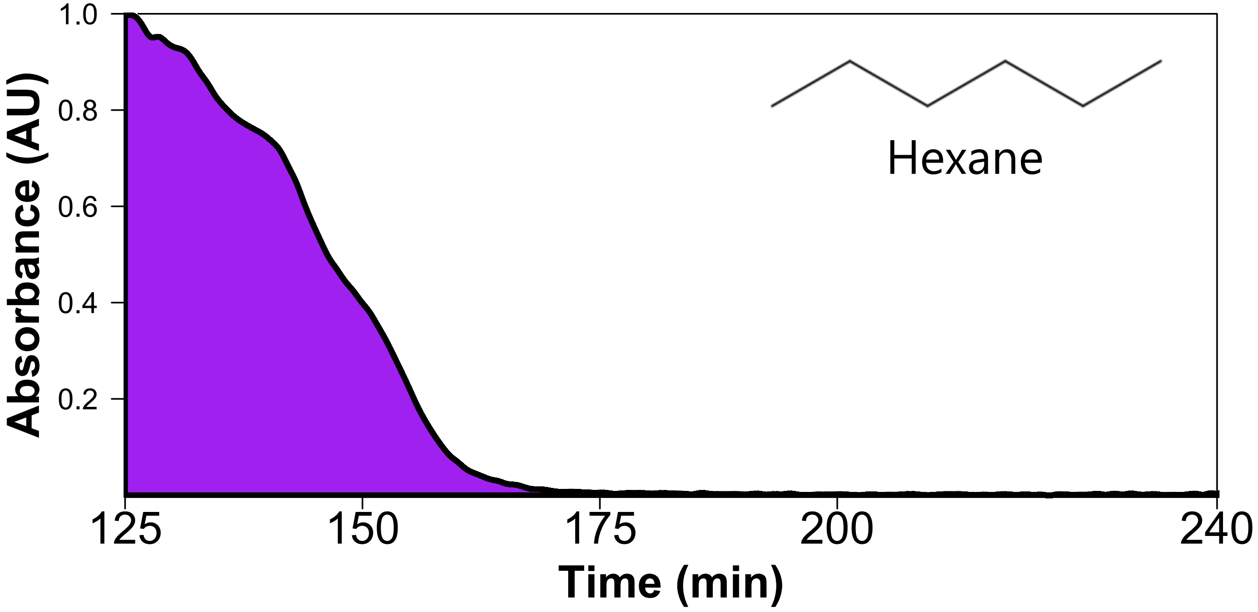
How Does VUV Spectroscopy Work?

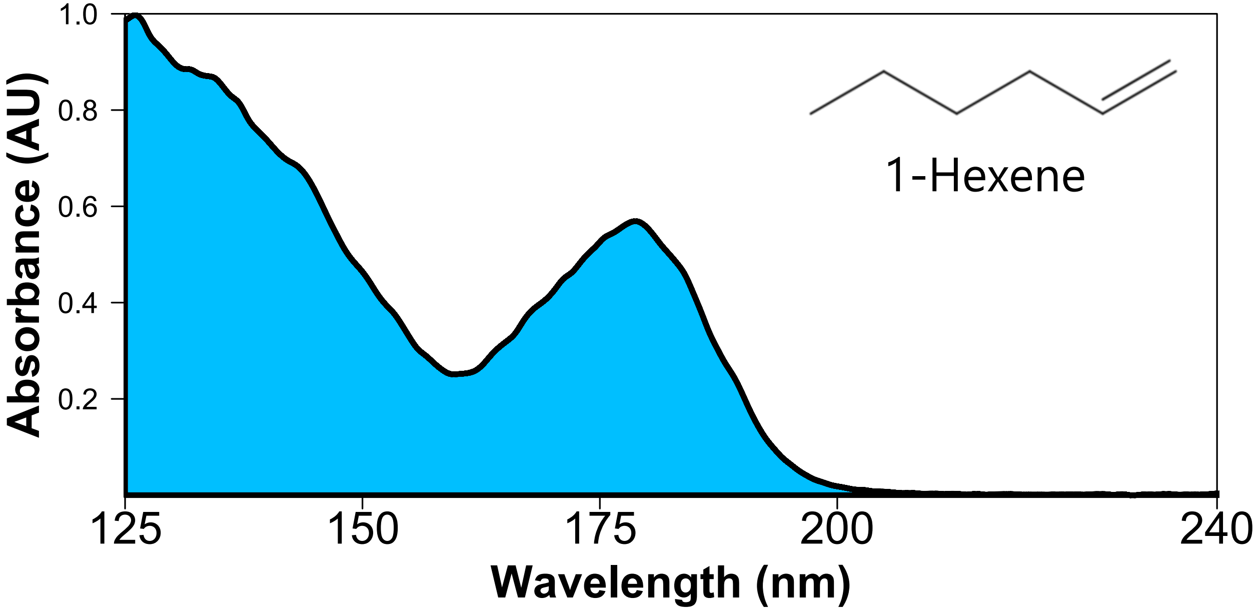


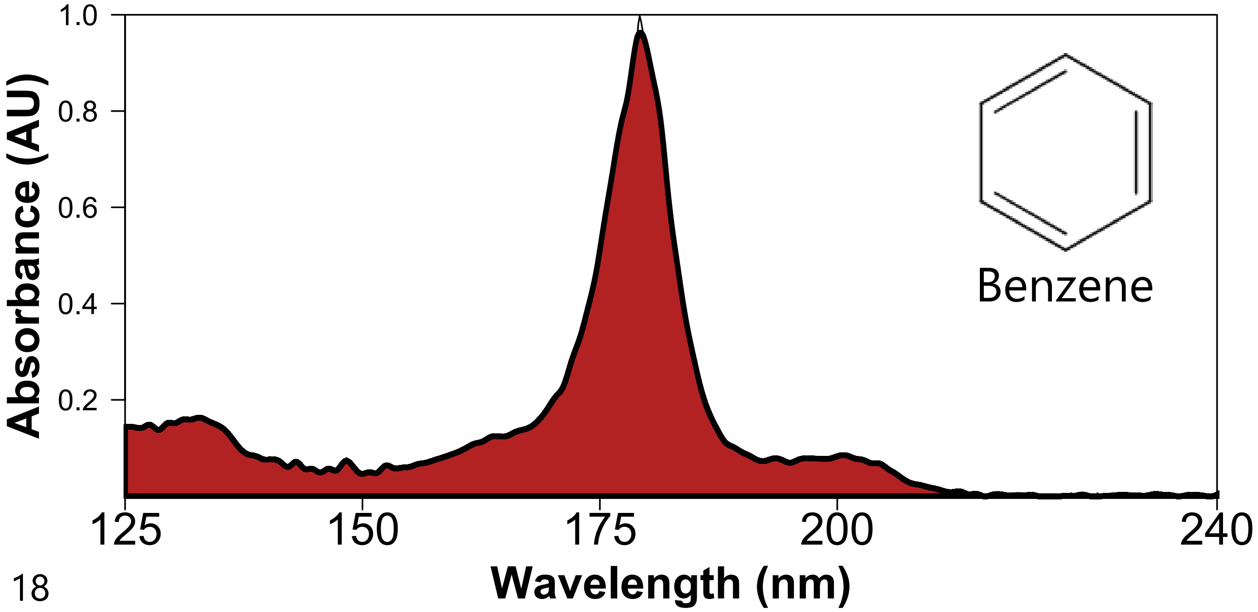
How Does VUV Spectroscopy Work?

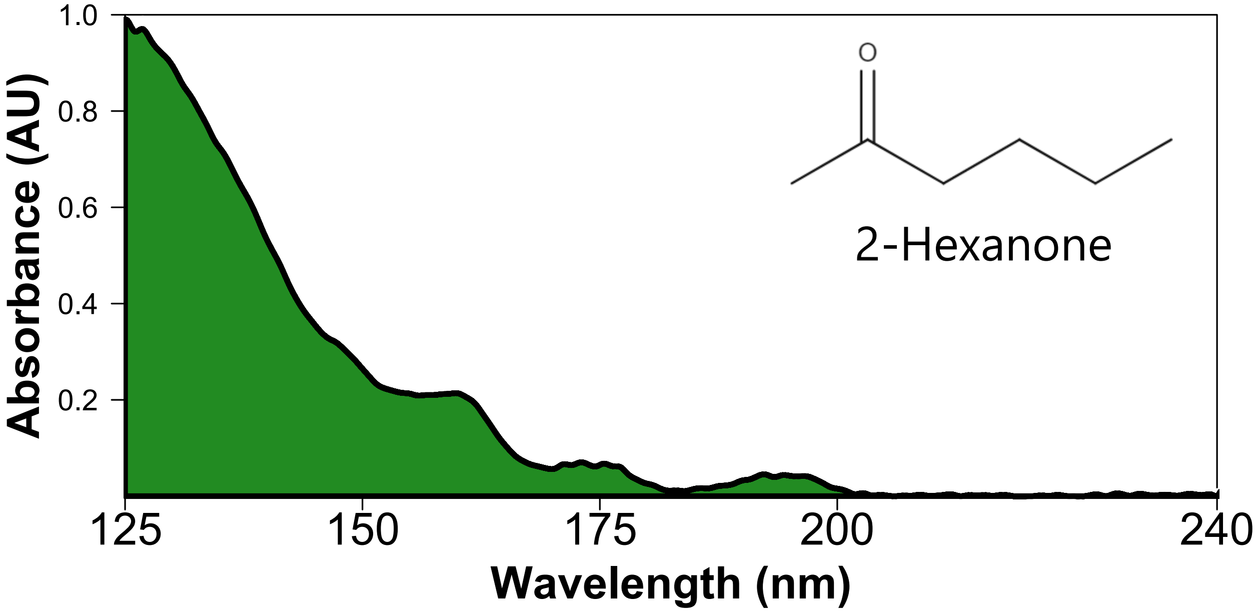


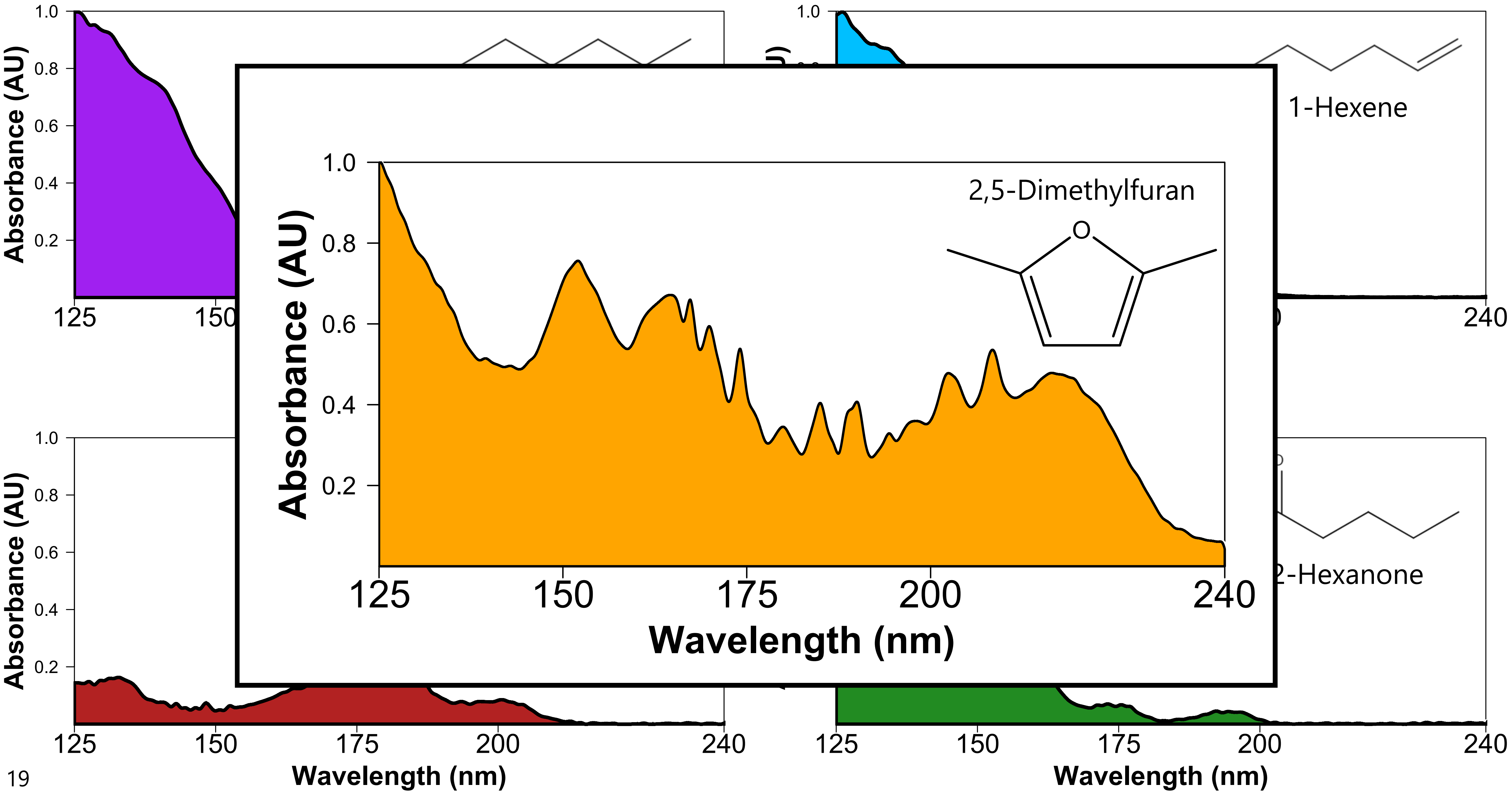


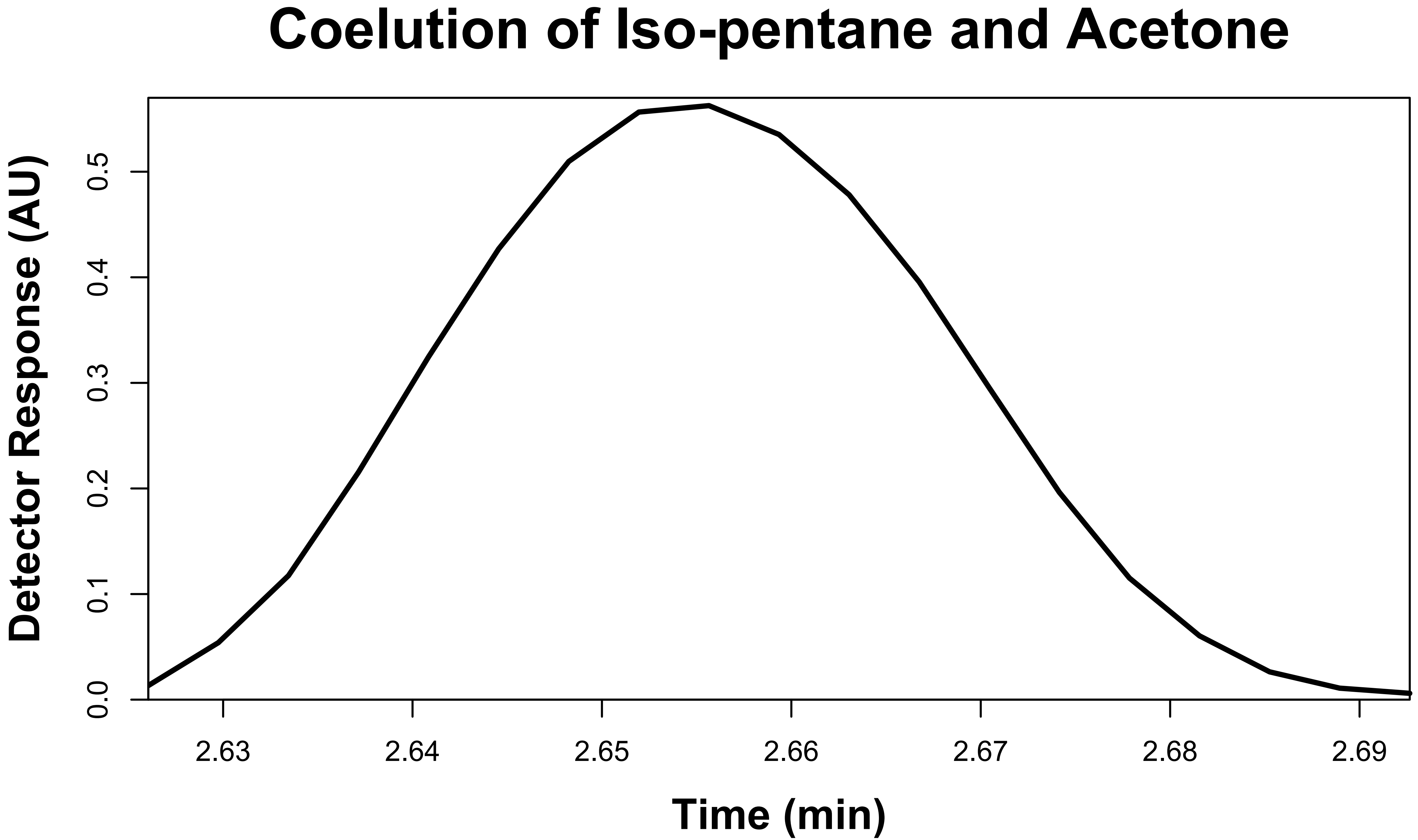

Hexane
Absorbance (AU)
1.0
0.8
0.6
0.4
0.2
125
150
175
200
240
Time (min)


1-Hexene
Absorbance (AU)
1.0
0.8
0.6
0.4
0.2
125
150
175
200
240
Wavelength (nm)

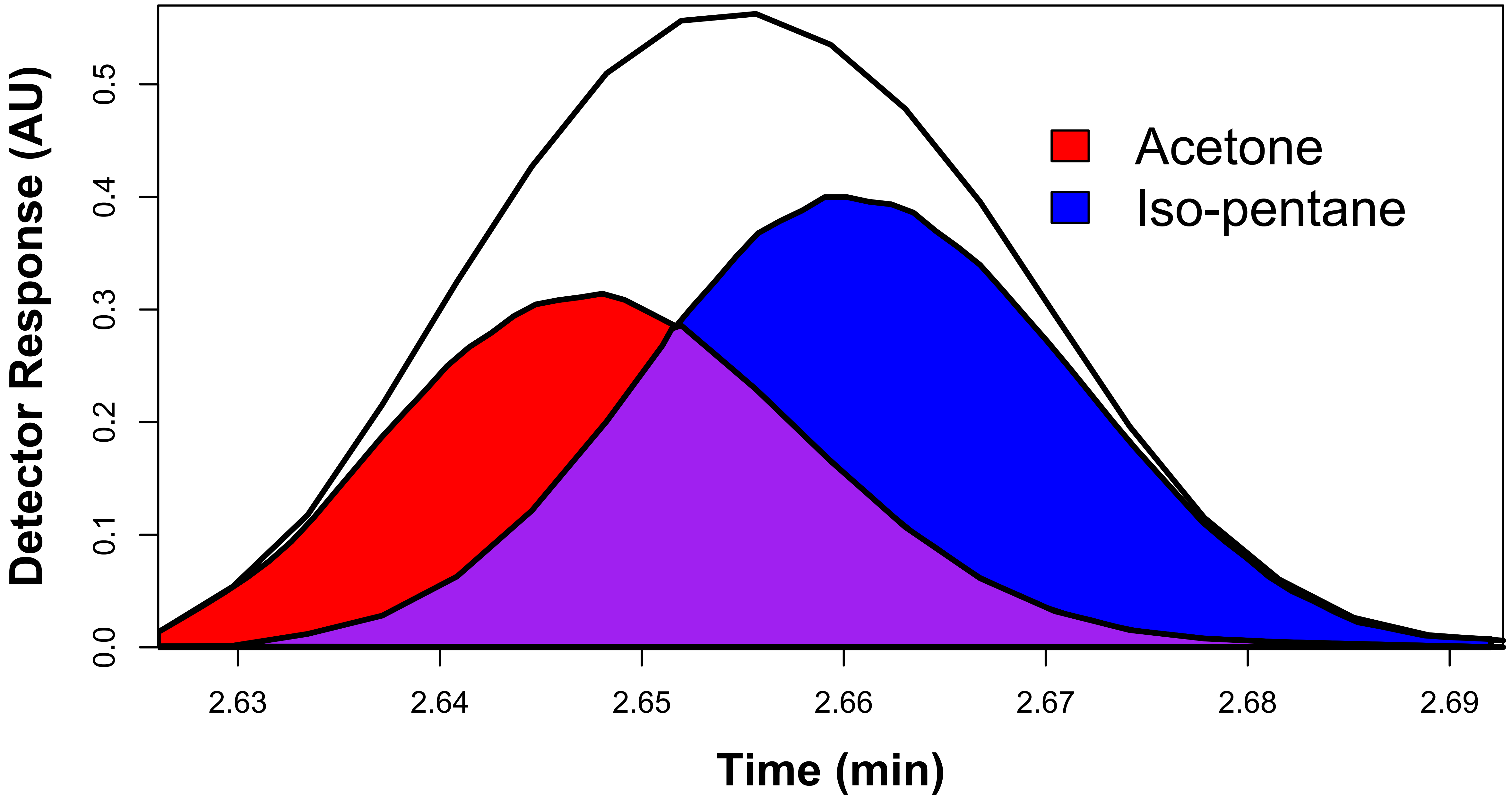

Benzene
Absorbance (AU)
1.0
0.8
0.6
0.4
0.2
125
150
175
200
240
Wavelength (nm)

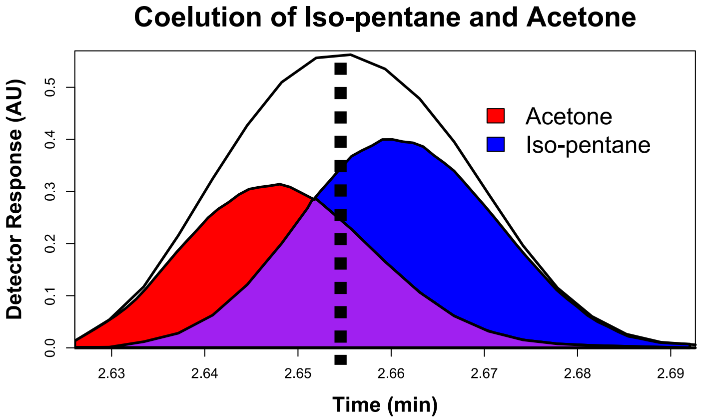

O
2-Hexanone
Absorbance (AU)
1.0
0.8
0.6
0.4
0.2
125
150
175
200
240
Wavelength (nm)

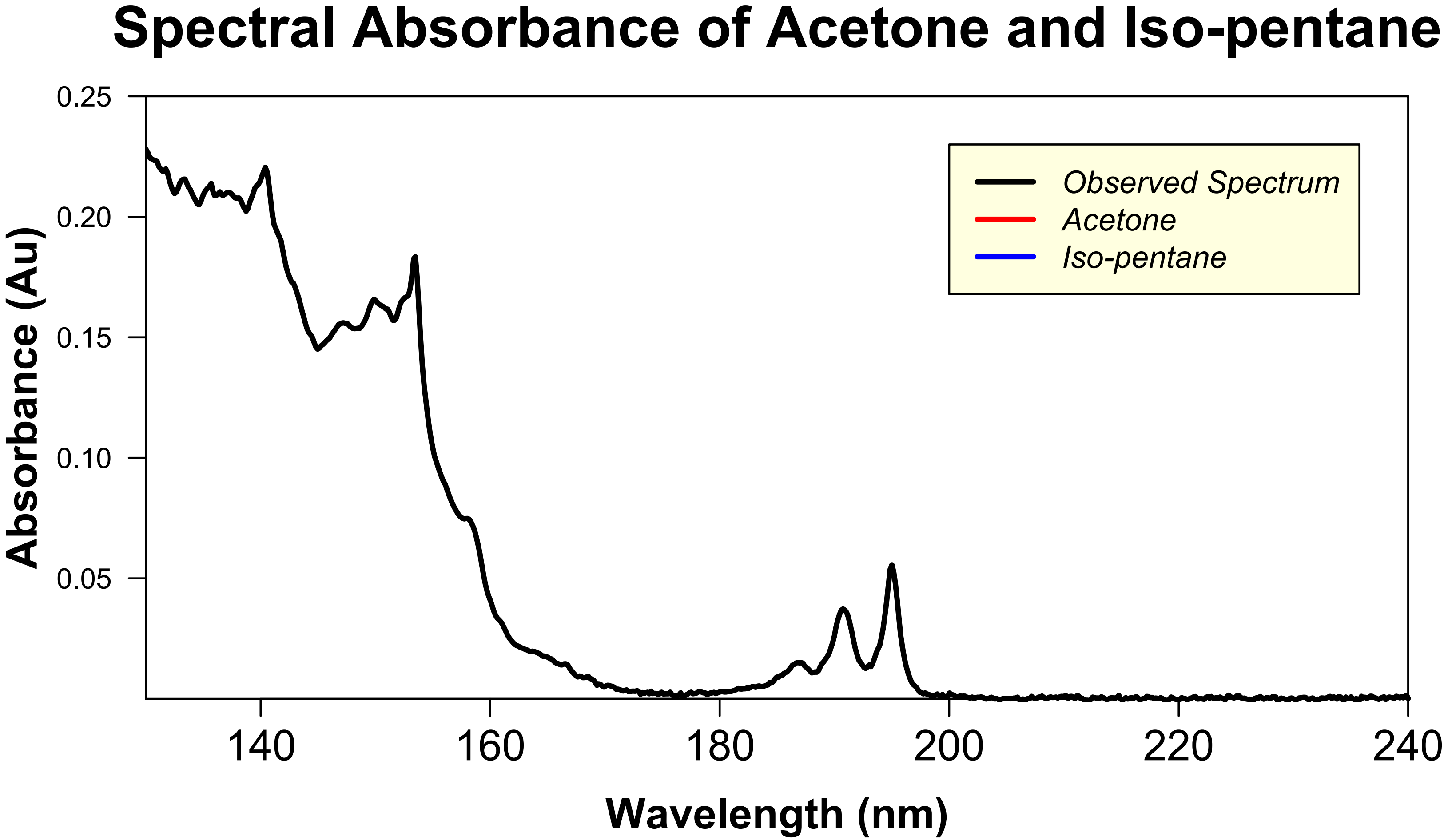

2,5-Dimethylfuran
O
1-Hexene
2-Hexanone
Absorbance (AU)
Wavelength (nm)
1.0
0.8
0.6
0.4
0.2
125
150
175
200
240

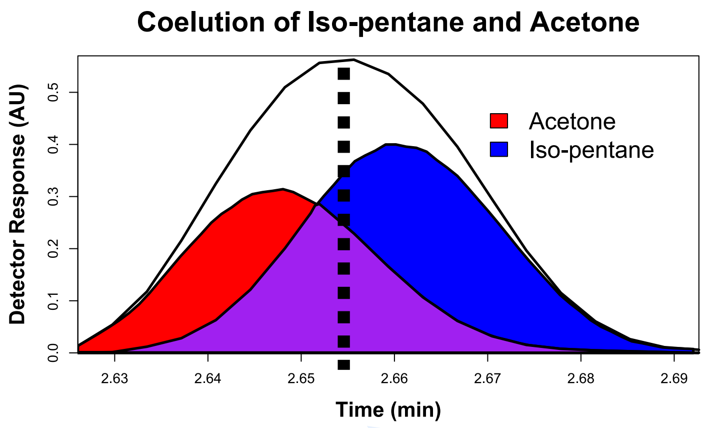

Coelution of Iso-pentane and Acetone
Detector Response (AU)
0.0
0.1
0.2
0.3
0.4
0.5
2.63
2.64
2.65
2.66
2.67
2.68
2.69
Time (min)

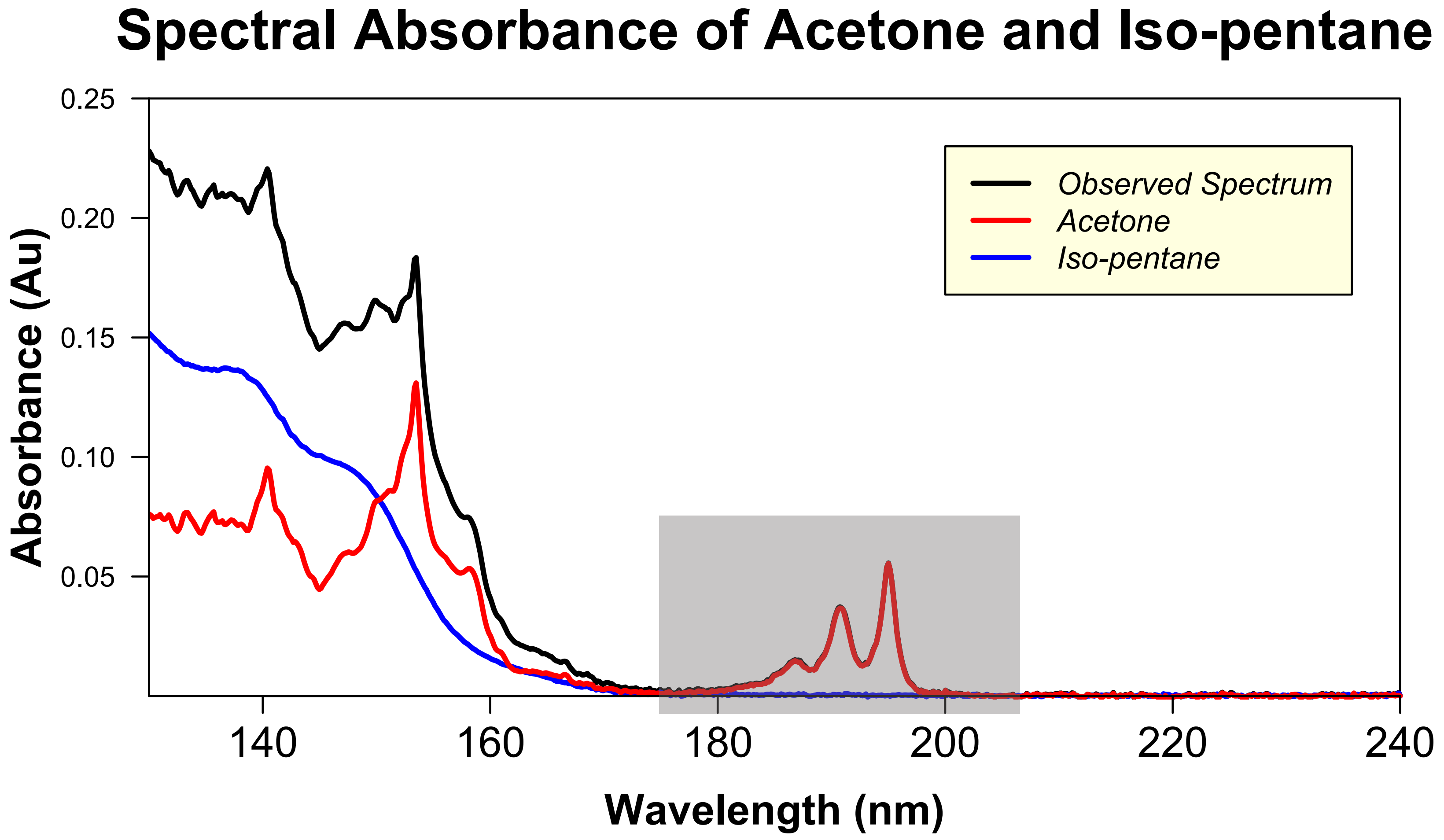
Coelution of Iso-pentane and Acetone




Coelution of Iso-pentane and Acetone
Detector Response (AU)
0.0
0.1
0.2
0.3
0.4
0.5
2.63
2.64
2.65
2.66
2.67
2.68
2.69
Time (min)
Acetone
Iso-pentane


Spectral Absorbance of Acetone and Iso-pentane
Absorbance (Au)
0.25
0.20
0.15
0.10
0.05
140
160
180
200
220
240
Wavelength (nm)
Observed Spectrum
Acetone
Iso-pentane


Coelution of Iso-pentane and Acetone
Detector Response (AU)
0.0
0.1
0.2
0.3
0.4
0.5
Acetone
Iso-pentane
2.63
2.64
2.65
2.66
2.67
2.68
2.69
Time (min)


Spectral Absorbance of Acetone and Iso-pentane
Absorbance (Au)
0.25
0.20
0.15
0.10
0.05
Observed Spectrum
Acetone
Iso-pentane
140
160
180
200
220
240
Wavelength (nm)

INTERNATIONAL

Designation: D8071 – 17

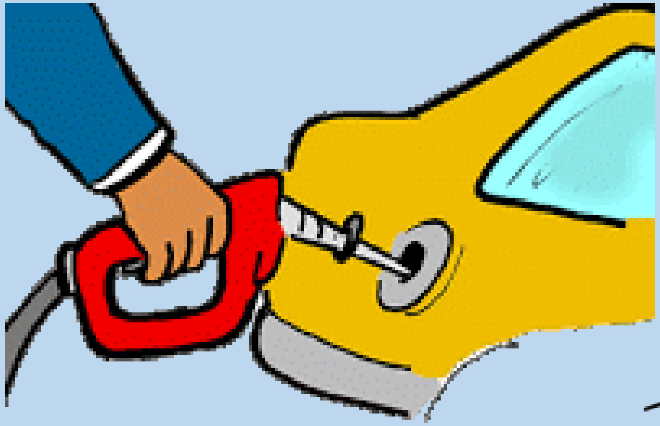
**Standard Test Method for
Determination of Hydrocarbon Group Types and Select Hydrocarbon and Oxygenate Compounds in Automotive Spark-Ignition Engine Fuel Using Gas Chromatography with Vacuum Ultraviolet Absorption Spectroscopy Detection (GC-VUV)[1]**

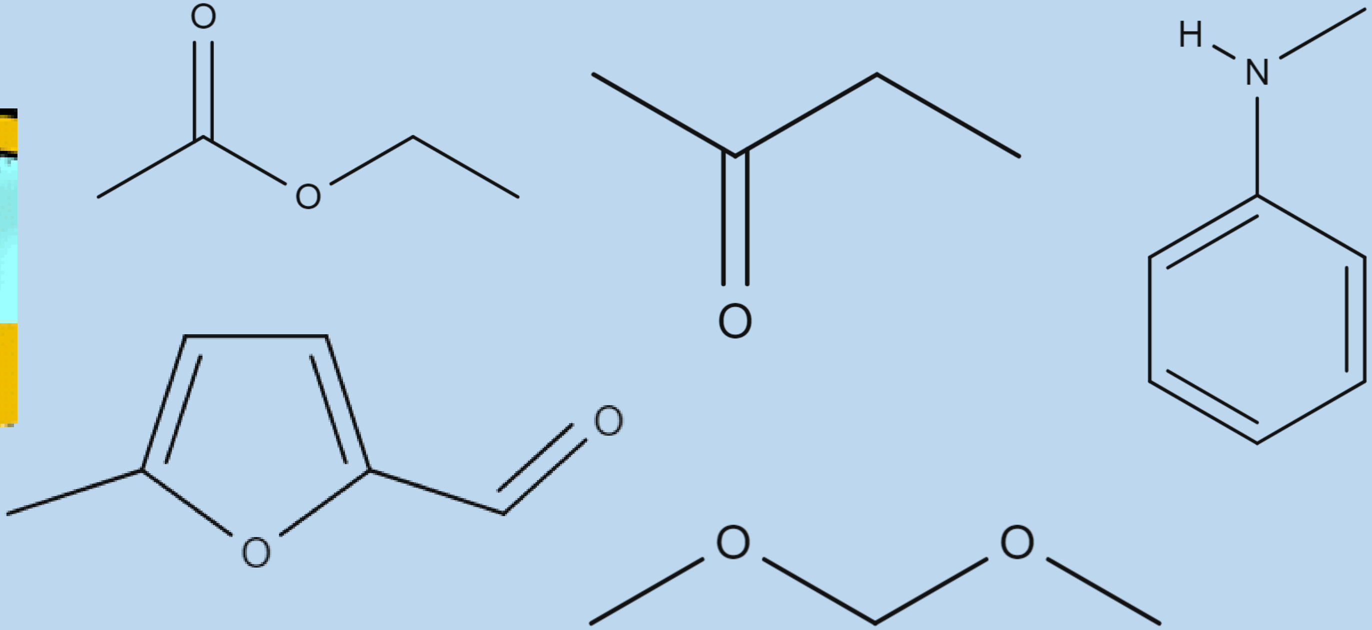
- ✓Under 35 minute run time
- ✓Identification by absorption and retention time
- ✓Spectral deconvolution
- ✓Easily add compounds to library

VUV ANALYTICS

Designation: D8071 – 17

Can we use ASTM D8071 conditions to analyze NTGAs?

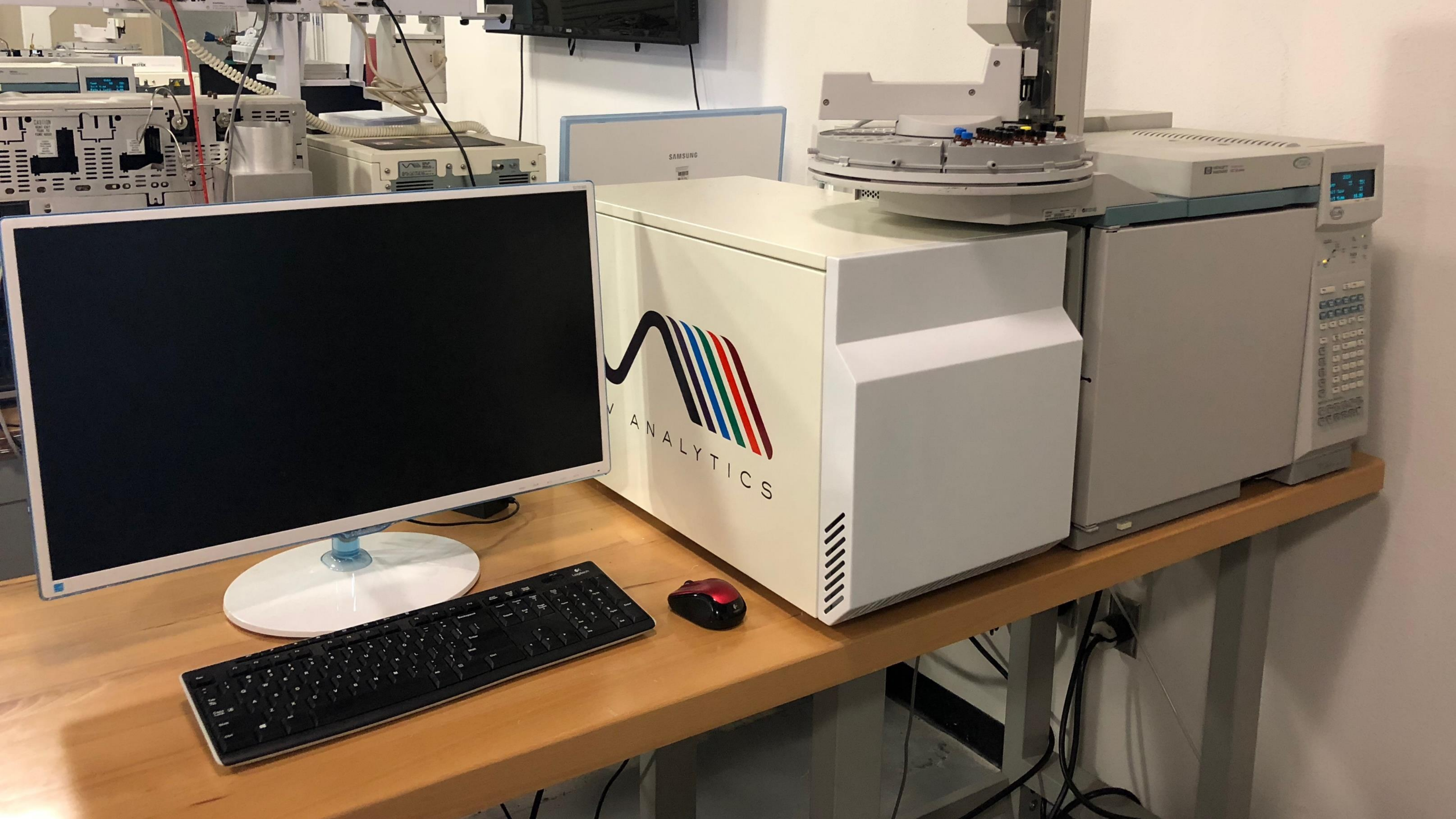




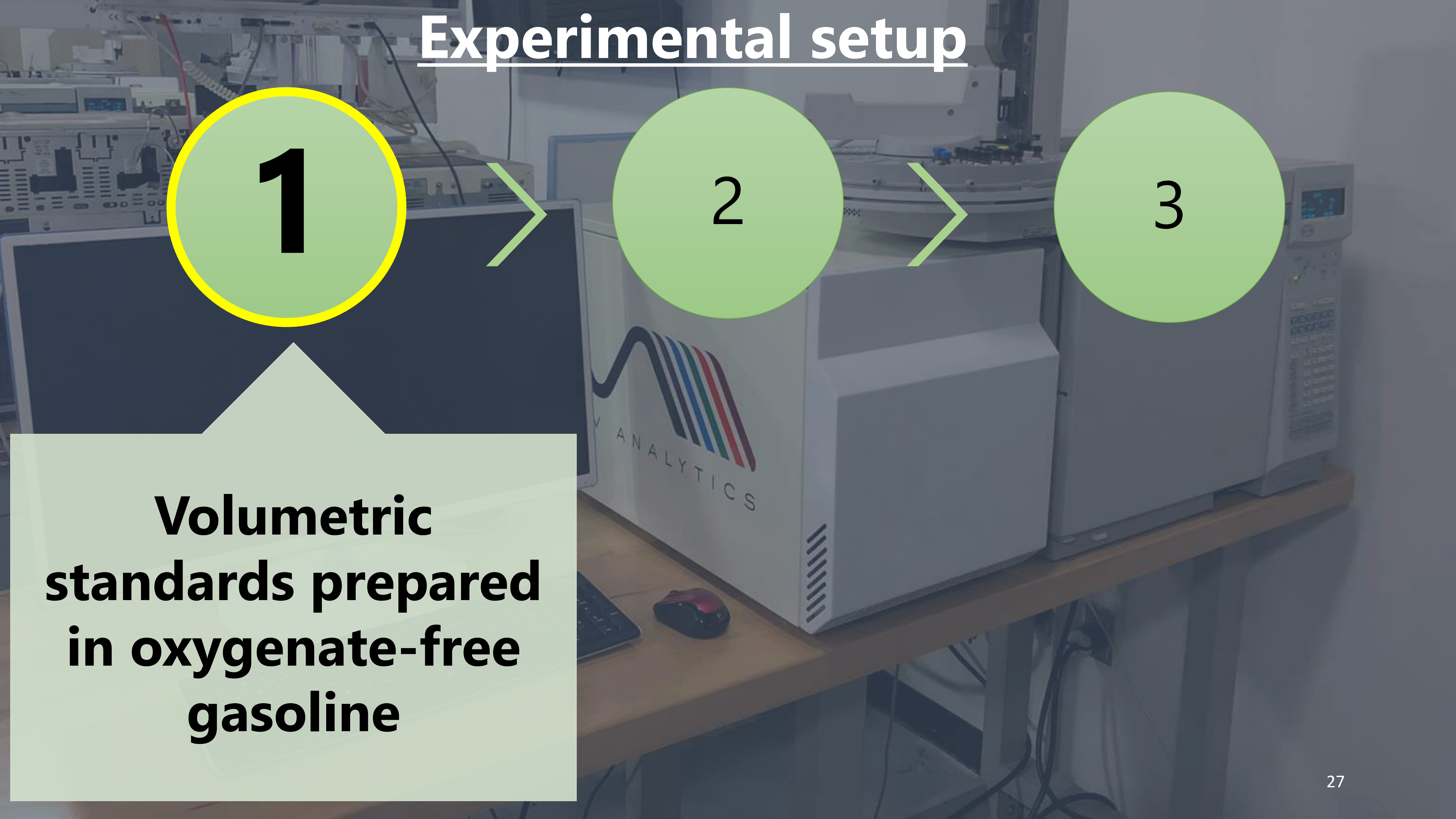
absorption and retention time

library

VUV ANALYTICS


ANALYTICS
SAMSUNG

Experimental setup



1 〉 2 〉 3

Volumetric standards prepared in oxygenate-free gasoline

Experimental setup

1

Volumetric standards prepared in oxygenate-free gasoline

Acetone	Isobutyl acetate
Dimethoxymethane	3-Hexanone
Methyl acetate	Diethyl carbonate
2-Butanone	2,4-Dimethyl-3-pentanone
2-Methylfuran	Ethyl butanoate
Dimethyl carbonate	n-Butyl acetate
Ethyl acetate	Methyl pentanoate
2-Methyltetrahydrofuran	Ethyl pentanoate
2-Pentanone	Anisole
2-Pentanol	Isobutyl isobutyrate
2,5-Dimethylfuran	gamma-Valerolactone
4-Methyl-2-Pentanone	Aniline
2-Methyl-1-butanol	Methyl levulinate
sec-Butyl acetate	Ethyl levulinate
Cyclopentanone	N-Methylaniline

1% 3% 5% 10%

Volume %

Experimental setup

1

Volumetric standards prepared in oxygenate-free gasoline

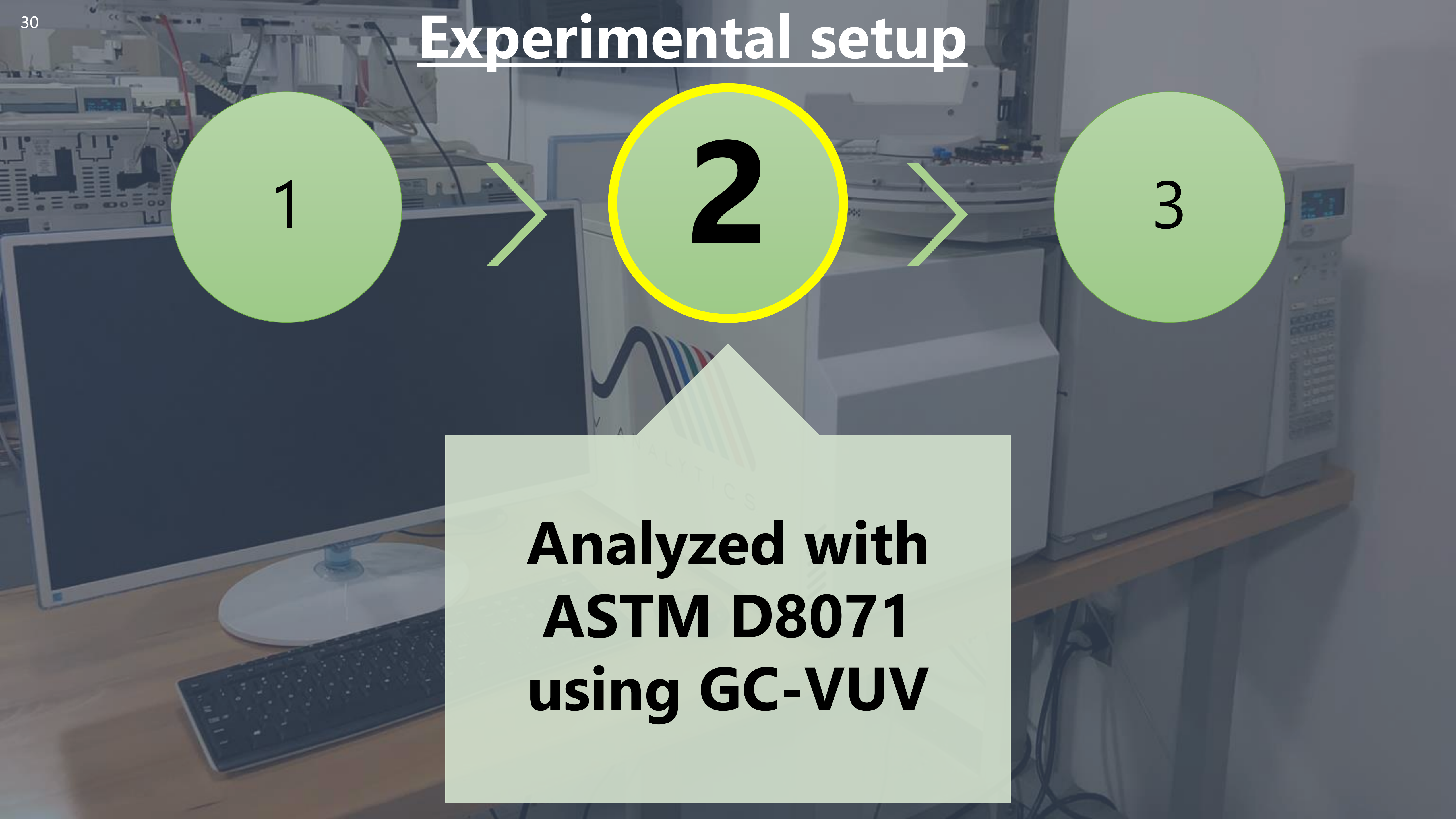
Acetone	Isobutyl acetate
Dimethoxymethane	3-Hexanone
Methyl acetate	Diethyl carbonate
2-Butanone	2,4-Dimethyl-3-pentanone
2-Methylfuran	Ethyl butanoate
Dimethyl carbonate	n-Butyl acetate
Ethyl acetate	Methyl pentanoate
2-Methyltetrahydrofuran	Ethyl pentanoate
2-Pentanone	Anisole
2-Pentanol	Isobutyl isobutyrate
2,5-Dimethylfuran	gamma-Valerolactone
4-Methyl-2-Pentanone	Aniline
2-Methyl-1-butanol	Methyl levulinate
sec-Butyl acetate	Ethyl levulinate
Cyclopentanone	N-Methylaniline

Additional samples:

0.05% 0.1% 0.2% 0.5%

1% 2% 5% 10% 20%

Experimental setup



1 › **2** › 3

Analyzed with ASTM D8071 using GC-VUV

Experimental setup

ASTM D8071

Agilent 6890 GC	*VUV Analytics VGA-100*
• Column: 30m x 0.25mm x 0.25µm Rxi-1ms • GC Inlet: 250°C, split 300:1 • Constant Flow Mode: 1.0 mL/min He • Injection volume: 1 µL • Oven: 35°C (10 min), 7°C/min to 200°C (0 min)	• Makeup gas: 0.25 psi N_2 • Acquisition range: 125-240 nm • Acquisition rate: 4.5 Hz • Detector flow cell: 275°C • Transfer line temperature: 275°C

Experimental setup

1 › 2 › **3**

A	=	Absorption
ε	=	Molar Absorptivity
b	=	Path Length
c	=	Concentration

Quantified

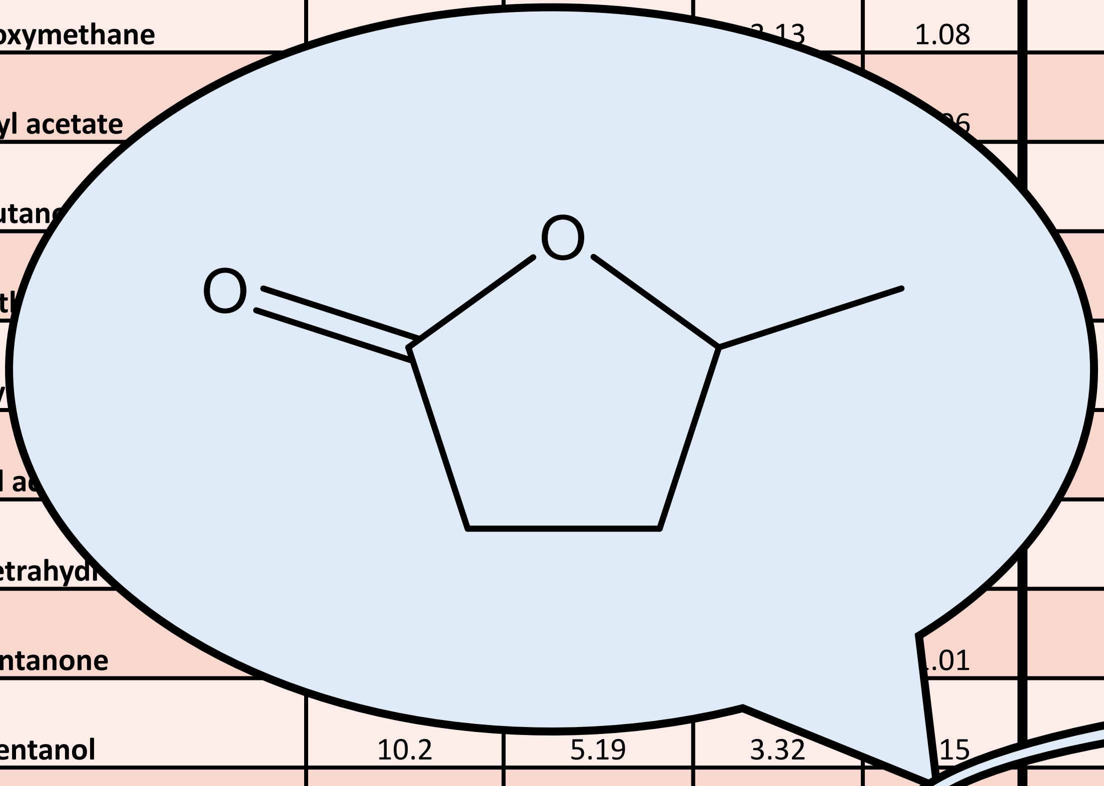
Beer-Lambert Law:

$$A = \varepsilon b c$$

NTGA Compound	10%	5%	3%	1%	NTGA Compound	10%	5%	3%	1%
Acetone	10.9	4.96	3.00	0.956	*Isobutyl acetate*	10.5	5.40	3.20	1.04
Dimethoxymethane	10.4	5.12	3.13	1.08	*3-Hexanone*	10.0	5.25	3.25	1.09
Methyl acetate	10.4	5.20	3.14	1.06	*Diethyl carbonate*	10.5	5.36	3.18	0.954
2-Butanone	10.4	5.12	3.09	1.11	*2,4-Dimethyl-3-pentanone*	10.1	5.15	3.18	1.08
2-Methylfuran	10.2	5.24	3.17	1.05	*Ethyl butanoate*	10.0	5.22	3.19	1.06
Dimethyl carbonate	10.5	5.21	3.09	1.05	*n-Butyl acetate*	10.2	5.27	3.16	1.06
Ethyl acetate	10.3	5.65	3.66	1.25	*Methyl pentanoate*	10.1	5.17	3.13	1.03
2-Methyltetrahydrofuran	10.2	5.13	3.13	1.04	*Ethyl pentanoate*	10.3	5.37	3.31	1.18
2-Pentanone	10.6	5.32	3.18	1.01	*Anisole*	10.1	5.16	3.03	1.04
2-Pentanol	10.2	5.19	3.32	1.15	*Isobutyl isobutyrate*	10.0	5.12	3.13	1.04
2,5-Dimethylfuran	10.2	5.18	3.18	1.03	*gamma-Valerolactone*	6.71	5.02	3.08	1.00
4-Methyl-2-Pentanone	10.3	5.30	3.19	1.06	*Aniline*	10.3	5.23	3.19	1.07
2-Methyl-1-butanol	10.3	5.38	3.21	1.08	*Methyl levulinate*	10.2	5.13	3.19	1.10
sec-Butyl acetate	10.5	5.43	3.25	1.08	*Ethyl levulinate*	10.2	5.20	3.16	1.06
Cyclopentanone	10.1	5.18	3.14	1.00	*N-Methylaniline*	10.3	5.32	3.28	1.08

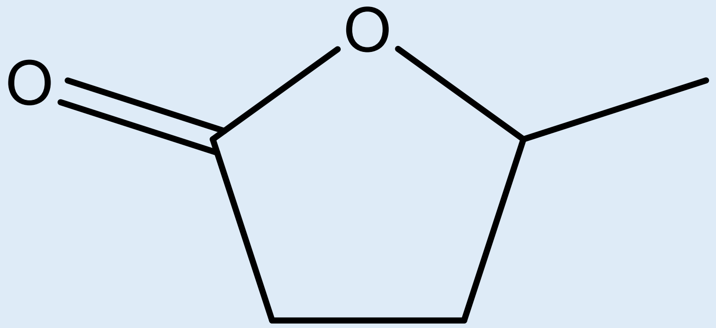
NTGA Compound	10%	5%	3%	1%
Acetone	10.9	4.96	3.00	0.956
Dimethoxymethane	[illegible]	[illegible]	[illegible]	1.08
Methyl acetate	[illegible]	[illegible]	[illegible]	[illegible]
2-Butan[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2-Met[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Dimethy[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Ethyl a[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2-Methyltetrahyd[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
2-Pentanone	[illegible]	[illegible]	[illegible]	[illegible]
2-Pentanol	10.2	5.19	3.32	[illegible]
2,5-Dimethylfuran	10.2	5.18	3.18	[illegible]
4-Methyl-2-Pentanone	10.3	5.30	3.19	1.06
2-Methyl-1-butanol	10.3	5.38	3.21	1.08
sec-Butyl acetate	10.5	5.43	3.25	1.08
Cyclopentanone	10.1	5.18	3.14	1.00

NTGA Compound	10%	5%	3%	1%
Isobutyl acetate	10.5	5.40	3.20	1.04
3-Hexanone	10.0	5.25	3.25	1.09
Diethyl carbonate	10.5	5.36	3.18	0.954
2,4-Dimethyl-3-pentanone	10.1	5.15	3.18	1.08
Ethyl butanoate	10.0	5.22	3.19	1.06
n-Butyl acetate	10.2	5.27	3.16	1.06
Methyl pentanoate	10.1	5.17	3.13	1.03
Ethyl pentanoate	10.3	5.37	3.31	1.18
Anisole	10.1	5.16	3.03	1.04
Isobutyl isobutyrate	10.0	5.12	3.13	[illegible]
gamma-Valerolactone	**6.71**	5.02	3.08	1.00
Aniline	10.3	5.23	[illegible]	1.07
Methyl levulinate	10.2	5.13	3.19	1.10
Ethyl levulinate	10.2	5.20	3.16	1.06
N-Methylaniline	10.3	5.32	3.28	1.08

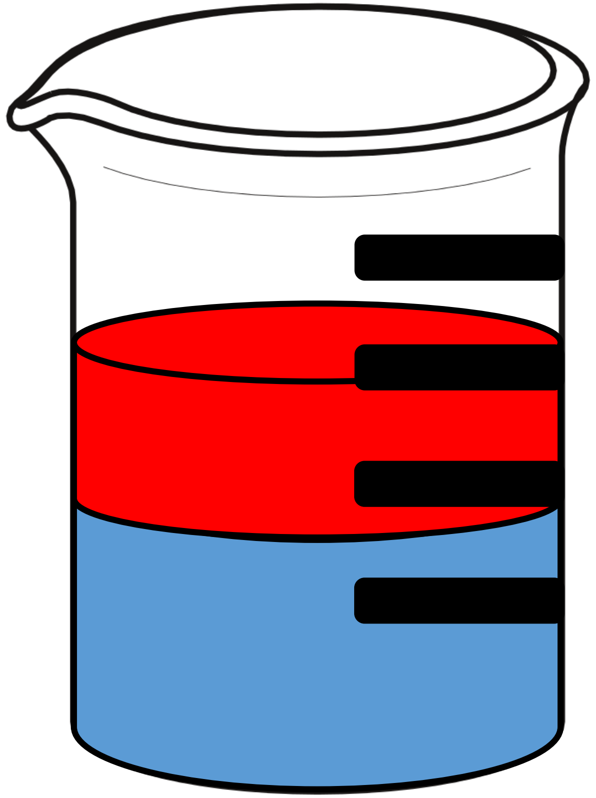


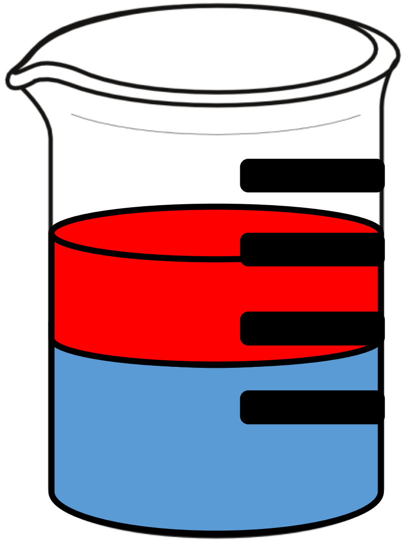
Oxygenate-Free Gasoline				
NTGA Compound	10%	5%	3%	1%
gamma-Valerolactone	**6.71**	5.02	3.08	1.00

gamma-Valerolactone



Insoluble





(No ethanol)
Insoluble

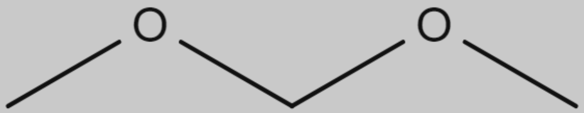
Oxygenate-Free Gasoline				
NTGA Compound	**10%**	**5%**	**3%**	**1%**
gamma-Valerolactone	**6.71**	5.02	3.08	1.00

(10% ethanol)
Soluble

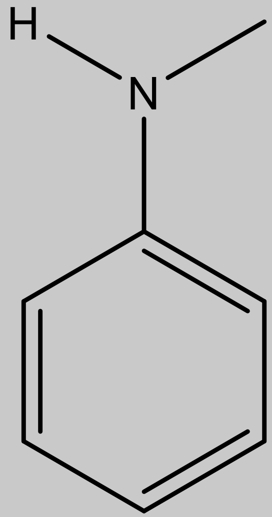
Murphy Express Gasoline				
NTGA Compound	**10%**	**5%**	**3%**	**1%**
gamma-Valerolactone	**10.3**	5.51	3.26	1.05

NTGA Compound	20%	10%	5%	2%	1%	0.5%	0.2%	0.1%	0.05%
Dimethoxymethane	20.9	9.85	4.90	1.83	1.00	0.49	0.22	0.09	0.06
N-Methylaniline	22.8	11.2	5.62	2.20	1.11	0.54	0.22	0.07	0.03
2,5-Dimethylfuran	20.7	9.96	4.88	1.83	1.01	0.47	0.16	0.06	0.02

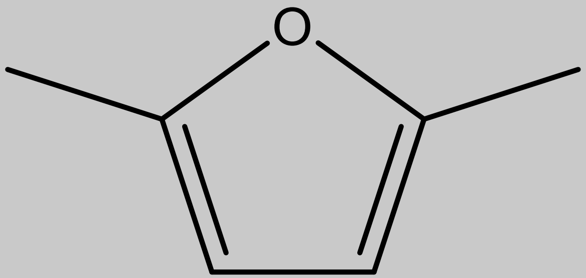
Dimethoxymethane



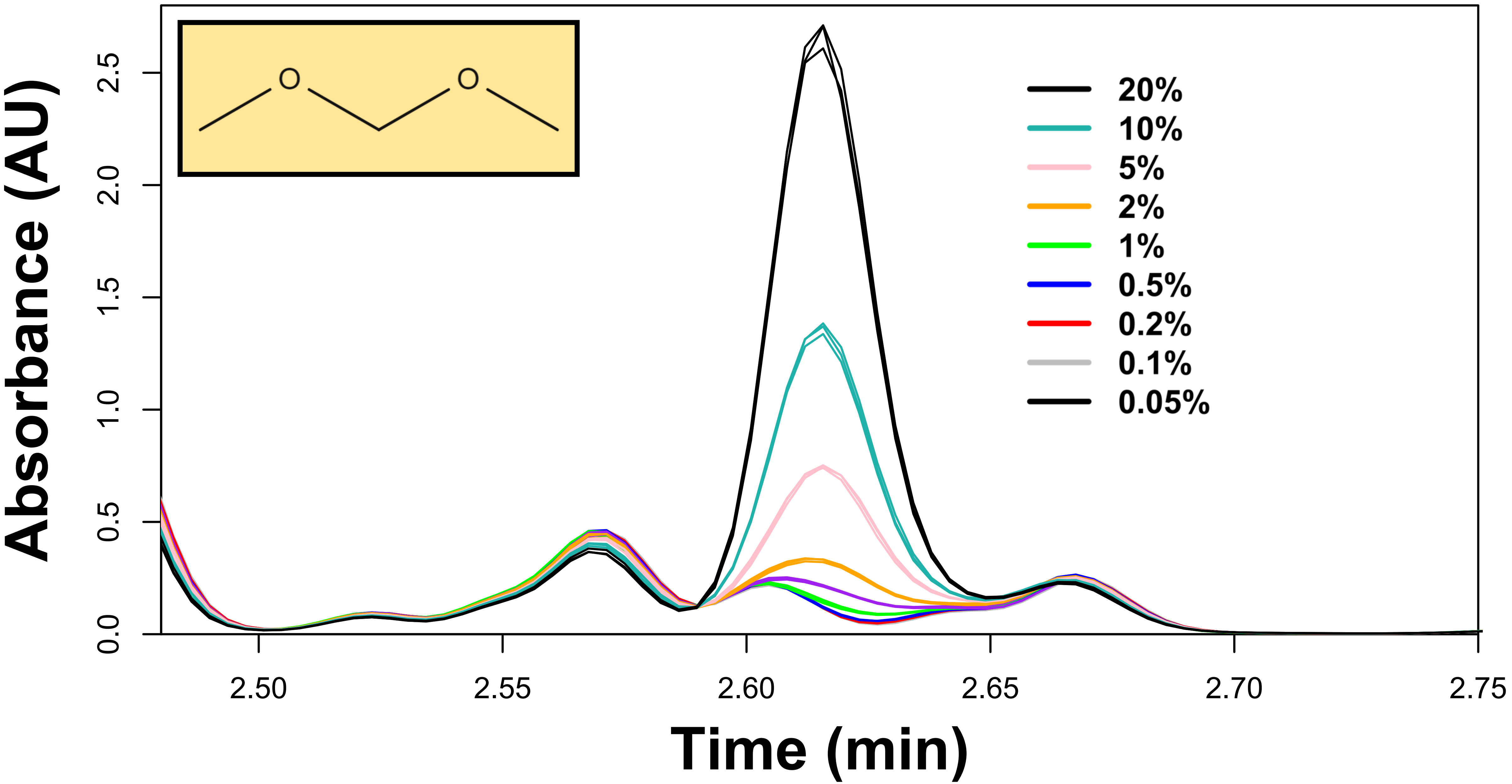
N-Methylaniline



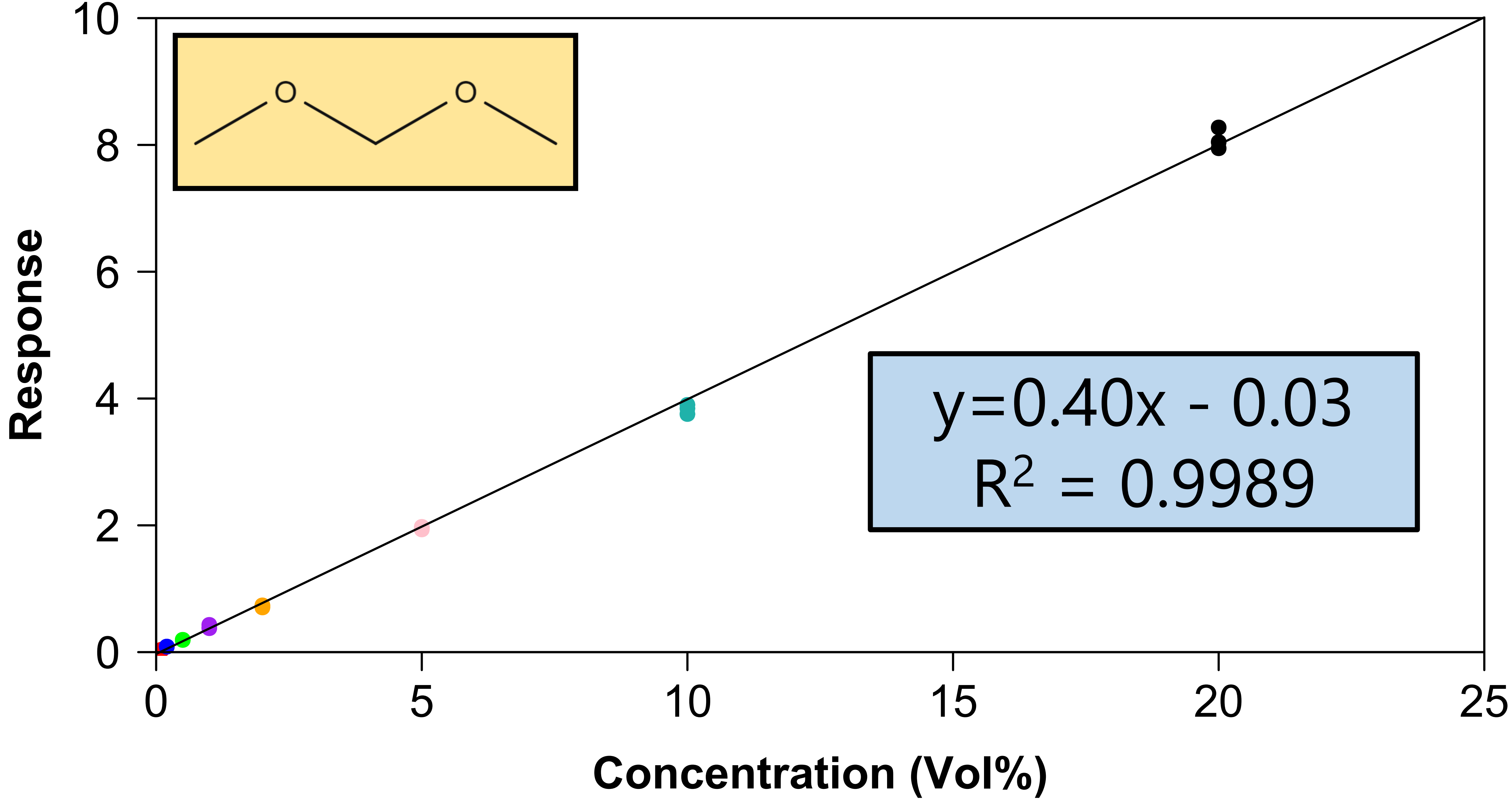
2,5-Dimethylfuran



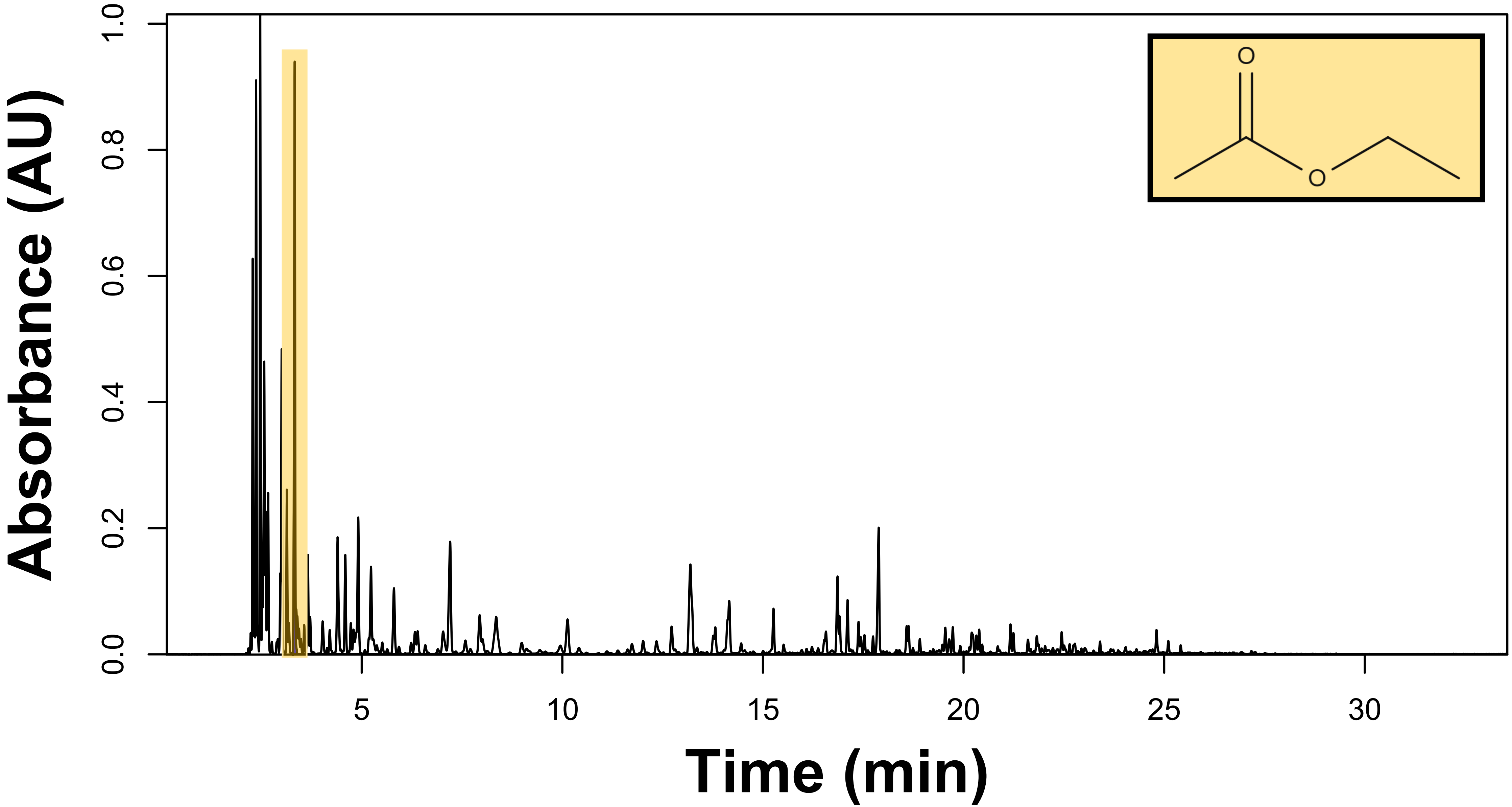
Dimethoxymethane in Gasoline

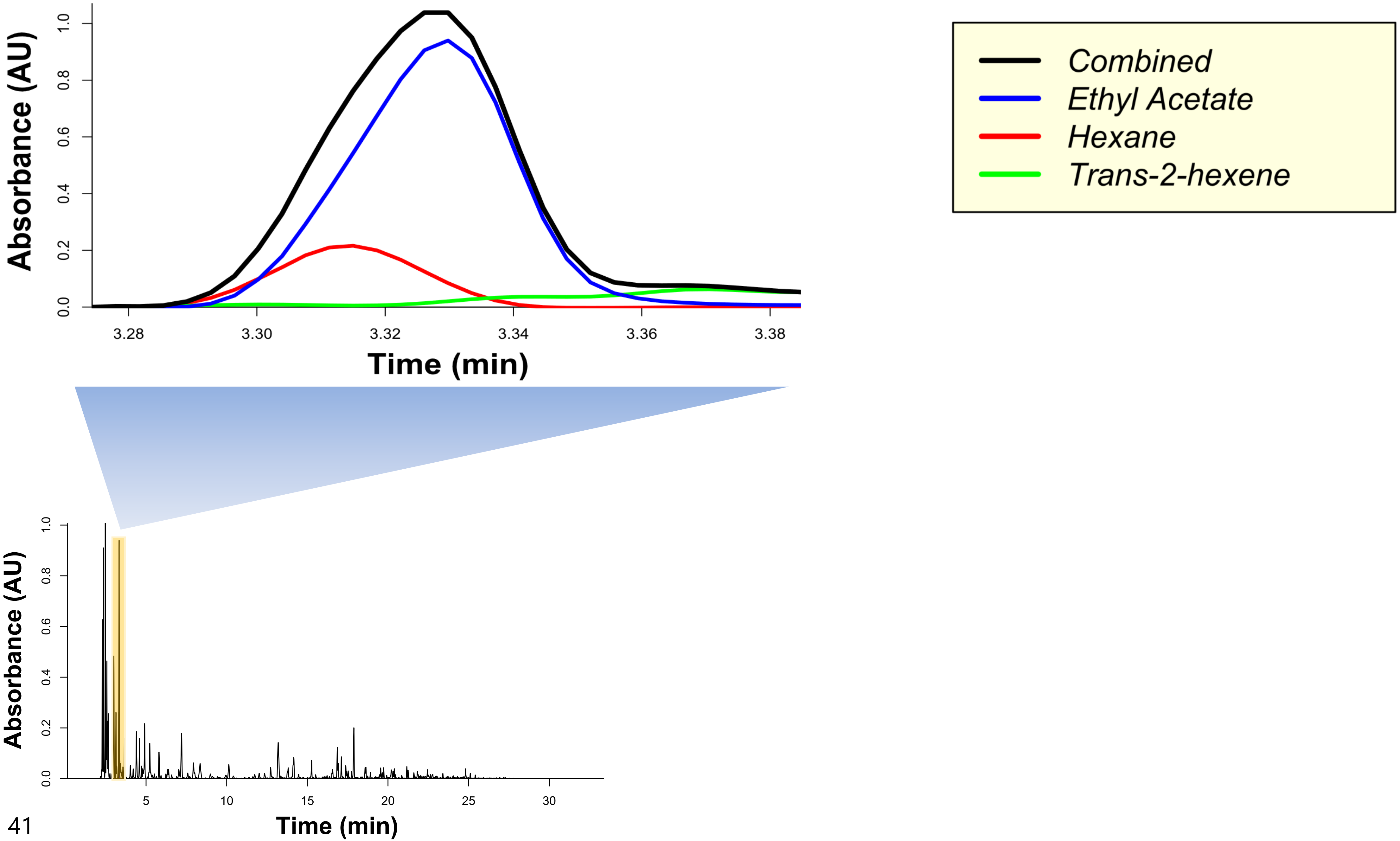


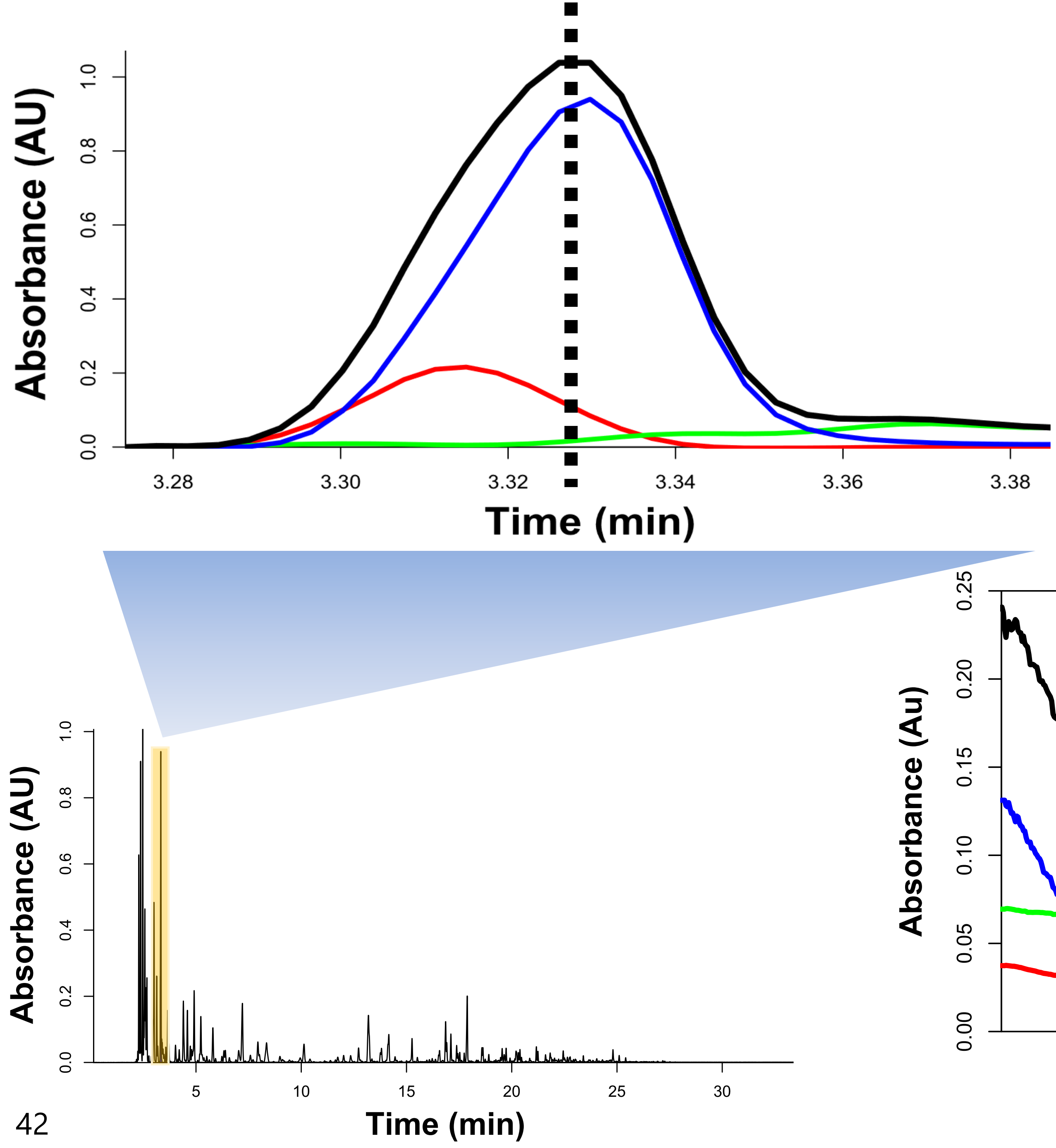
Dimethoxymethane Response vs. Concentration %

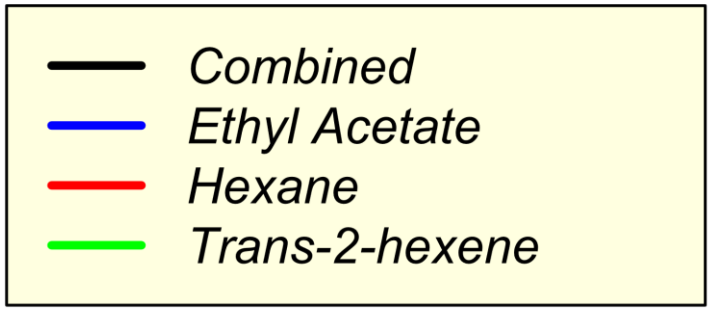


10% Ethyl Acetate in Gasoline

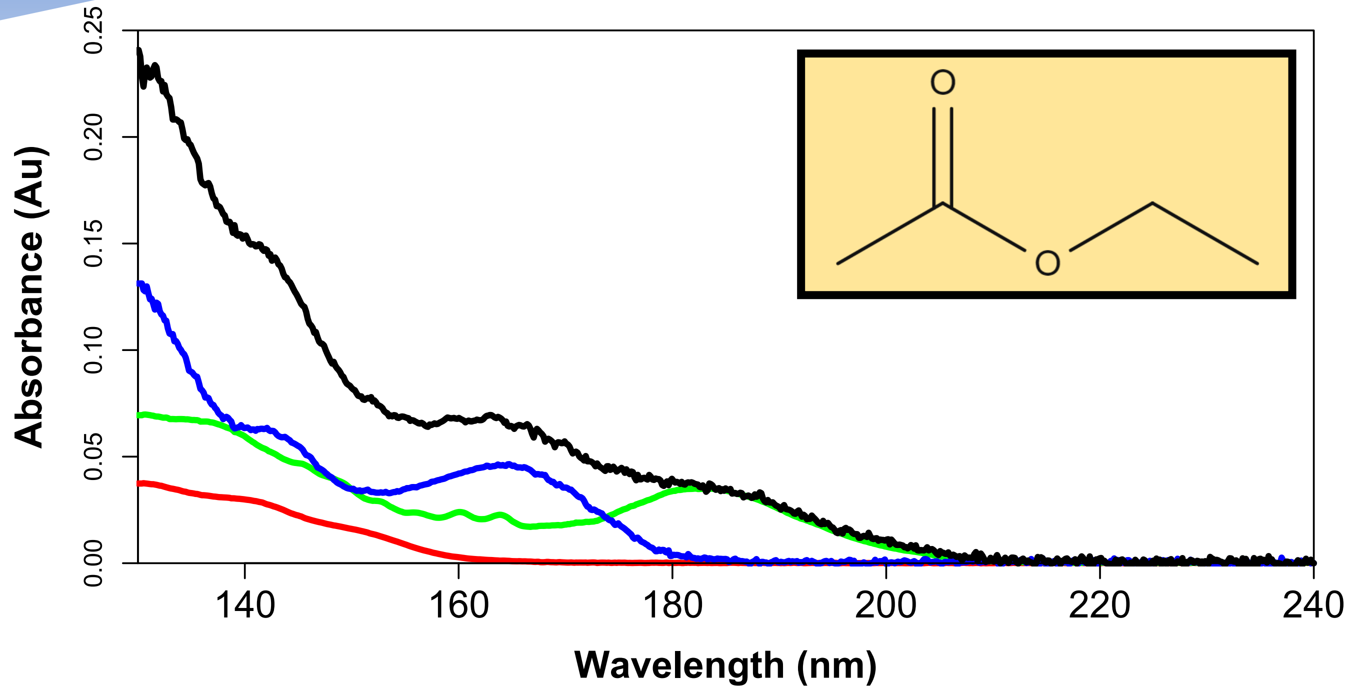



Absorbance (AU)
Time (min)
Combined
Ethyl Acetate
Hexane
Trans-2-hexene
Absorbance (AU)
Time (min)





Spectral Deconvolution of Ethyl Acetate



Conclusions

- NTGAs can be analyzed using GC-VUV and ASTM D8071 conditions
  - Compounds easily added to library
  - Deconvolve coeluting compounds
  - Accurately quantified

- ASTM D8071 conditions are favorable over ASTM D6730
  - Shorter run time
  - Confidence in identification
  - No method changes necessary

VUV ANALYTICS

Image: https://www.videoblocks.com/video/oil-platform-at-sea-at-sunset-lkqbl2d

Questions?

Ryan.Schonert@VUVanalytics.com