



## Characterization of the DiscoverIR-GC

**Instrumentation** DiscoverIR-GC  
Agilent 6890 GC with 7683B Autosampler  
Agilent ChemStation software running the GC and autosampler

<b>Samples</b>	Vial 5	3,000 $\mu\text{g/mL}$ each component in $\text{CHCl}_3$		
	Vial 4	300 $\mu\text{g/mL}$	"	
	Tetradecane	Vial 3	90 $\mu\text{g/mL}$	"
	Vanillin acetate	Vial 2	60 $\mu\text{g/mL}$	"
	Caffeine	Vial 1	30 $\mu\text{g/mL}$	"
	Vial 0	Chloroform solvent		

**GC conditions**

DB-5 column	15 m x 0.25mm ID x 0.25 $\mu\text{m}$ film thickness
Column temperature	240 $^{\circ}\text{C}$ isothermal
Injector and transfer lines	250 $^{\circ}\text{C}$
Sample disk	-40 $^{\circ}\text{C}$
Carrier gas	Helium constant flow, 1.2 mL/min
Split ratio	1:30

**Experiment** The DiscoverIR collected data as a single chromatographic run.  
The Agilent autosampler made the following sequence of injections at intervals of 2.10 minutes:

Duplicate injections from	Vials 5, 4, 3, 2, and 1
Triplicate injections from the blank	Vial 0
Single injections from	Vials 1, 2, 3, 4, and 5
Single injection solvent blank	Vial 0

**Data workup** The DiscoverIR software collected spectra at  $\frac{1}{2}$  second intervals. The most intense spectrum from each chromatographic peak was used for the calculations. The Tabulate Spectrum program, which is a standard feature of the DiscoverIR software, calculated peak heights of the most intense IR bands from each spectrum, writing these intensities and band positions to an Excel file. The chromatograms and spectra were plotted from Grams. The graphs of the data were plotted directly from Excel.

**Results** Linear range over two orders of magnitude ( 1 to 100 ng on-column)  
Average standard deviation from triplicate readings:  
**Tetradecane 9%, Vanillin acetate 12%, Caffeine 5%**  
Signal-to-noise ratio on-the-fly from the lowest concentration (1 ng) samples  
**Tetradecane 60 S/N, Vanillin acetate 15 S/N, Caffeine 15 S/N**

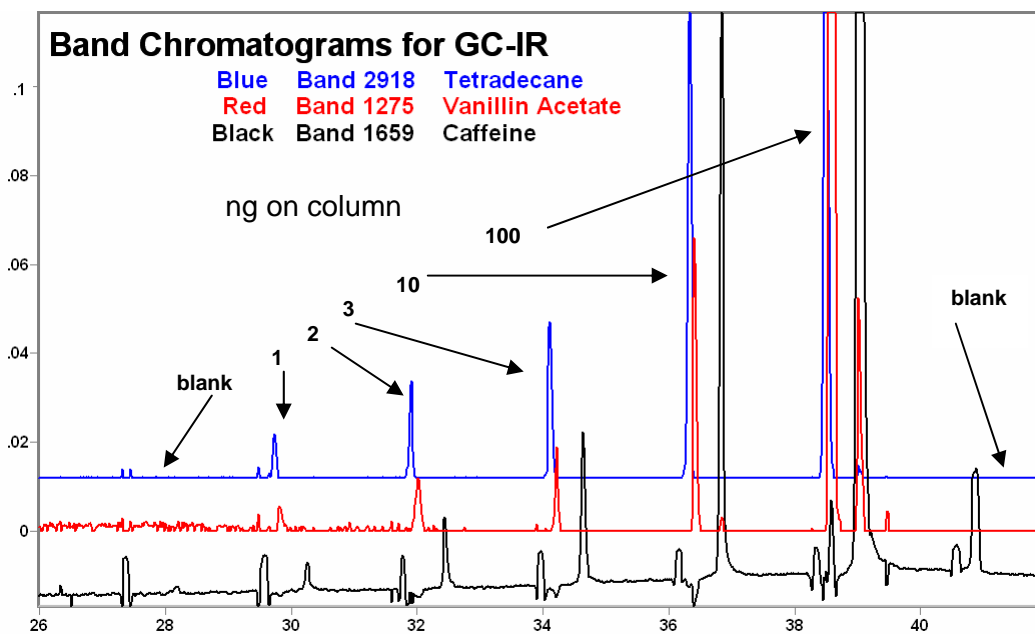
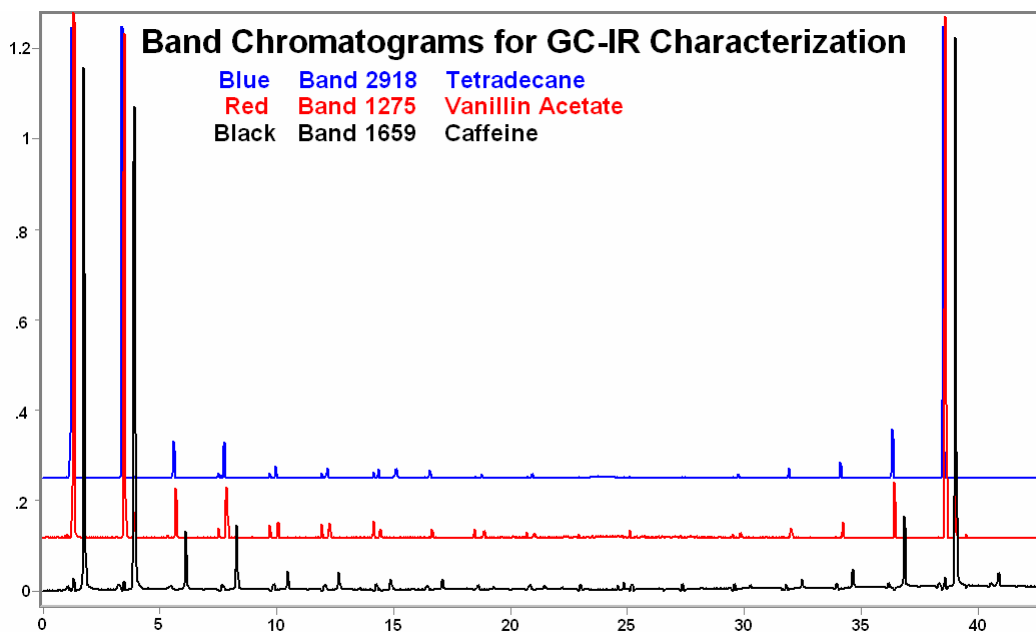




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## Application Note 015

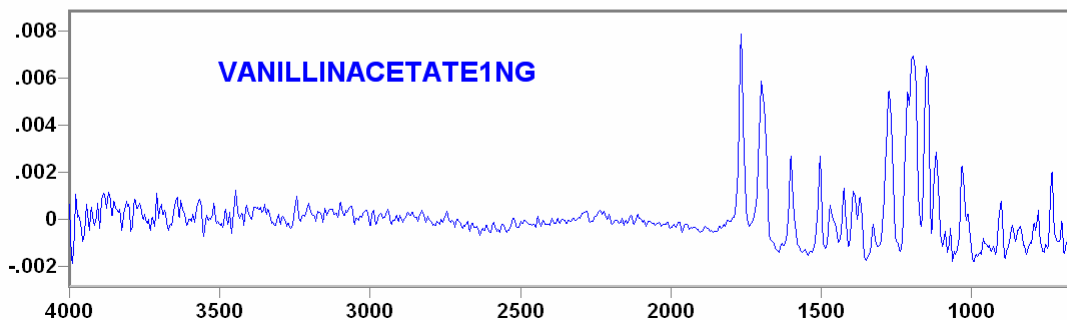
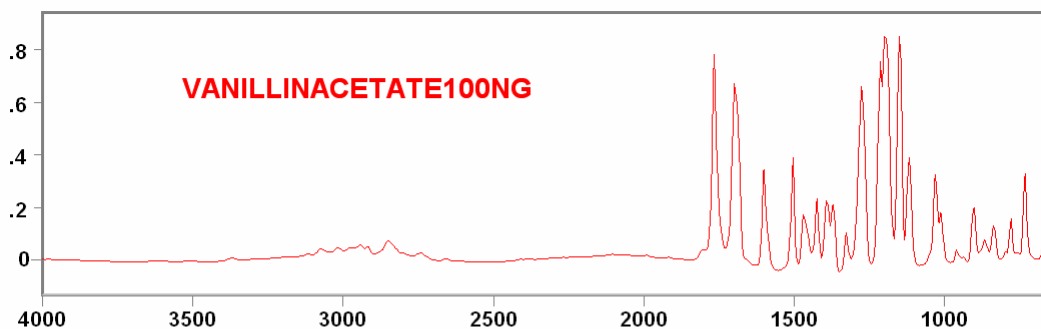
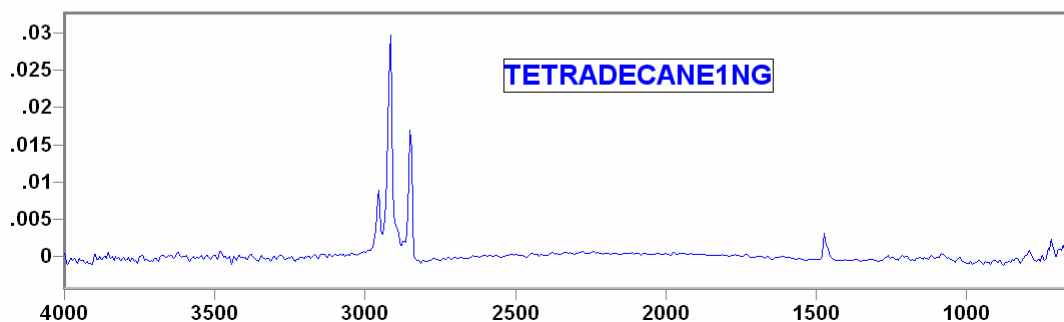
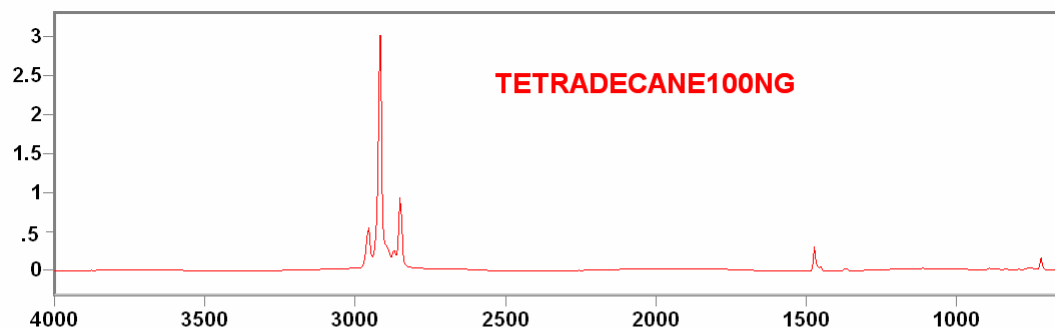
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Typical spectra from highest and lowest concentrations

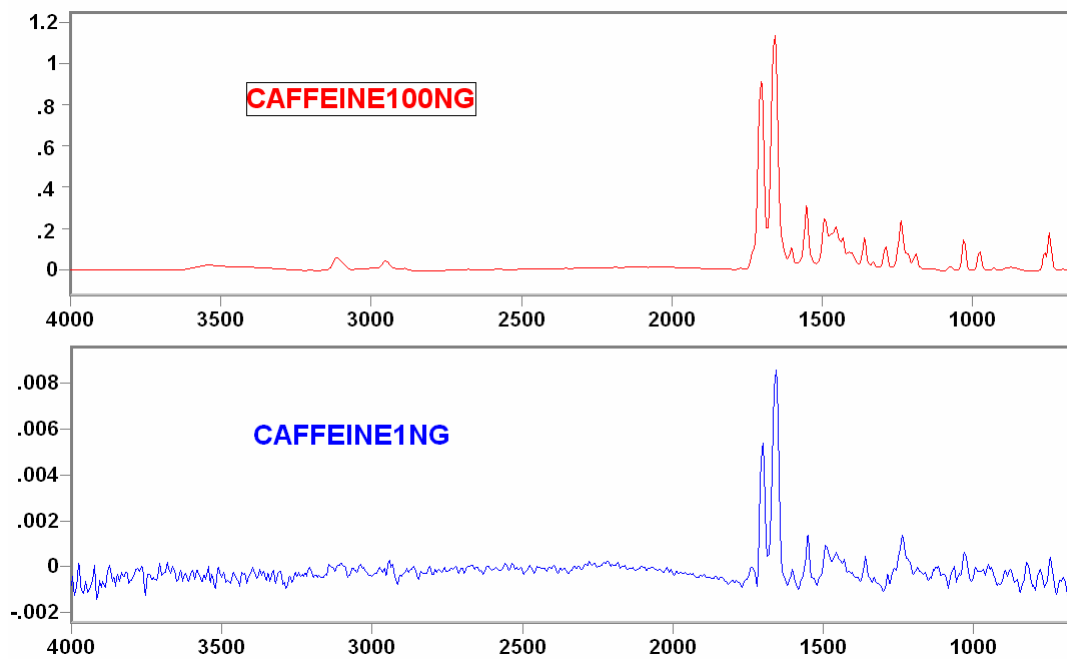




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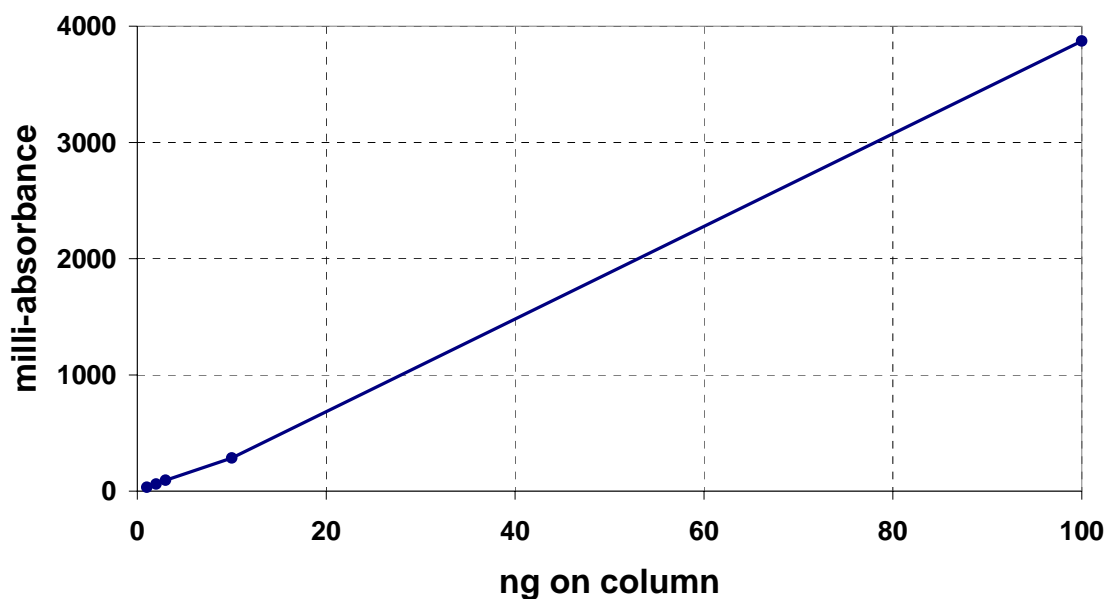


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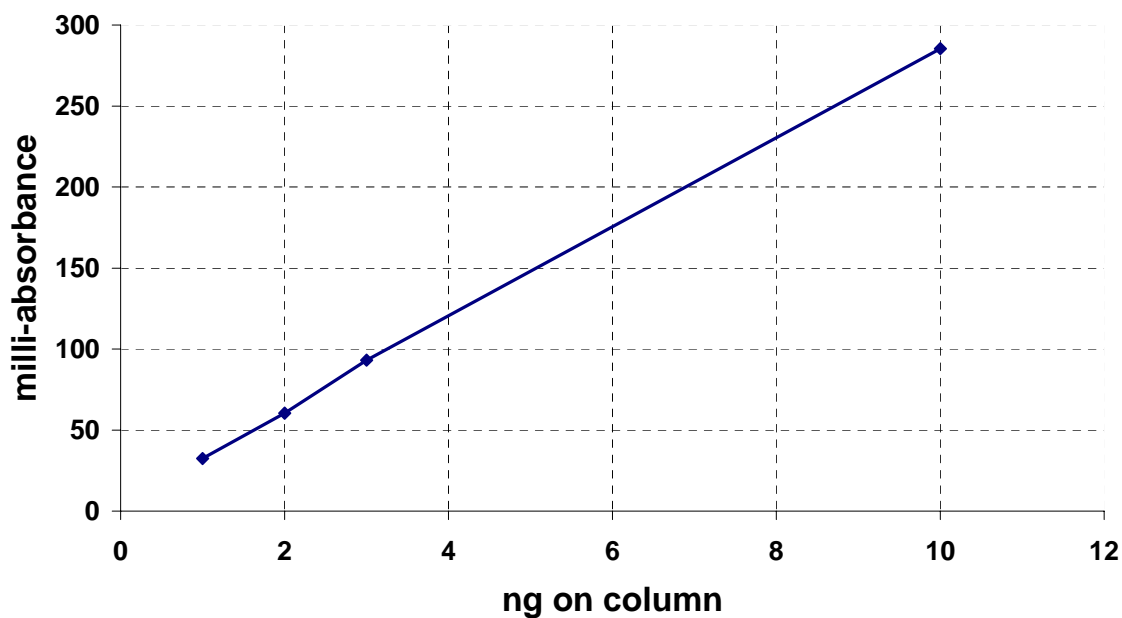
## Tetradecane Band 2918

Each point is the average of three measurements



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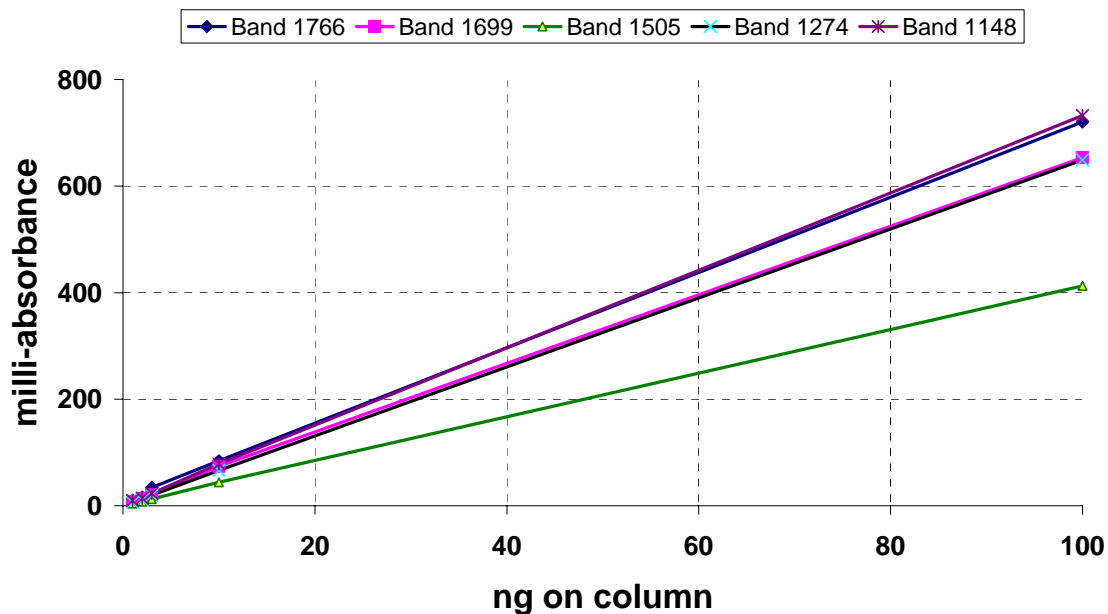
Each point is the average of three measurements





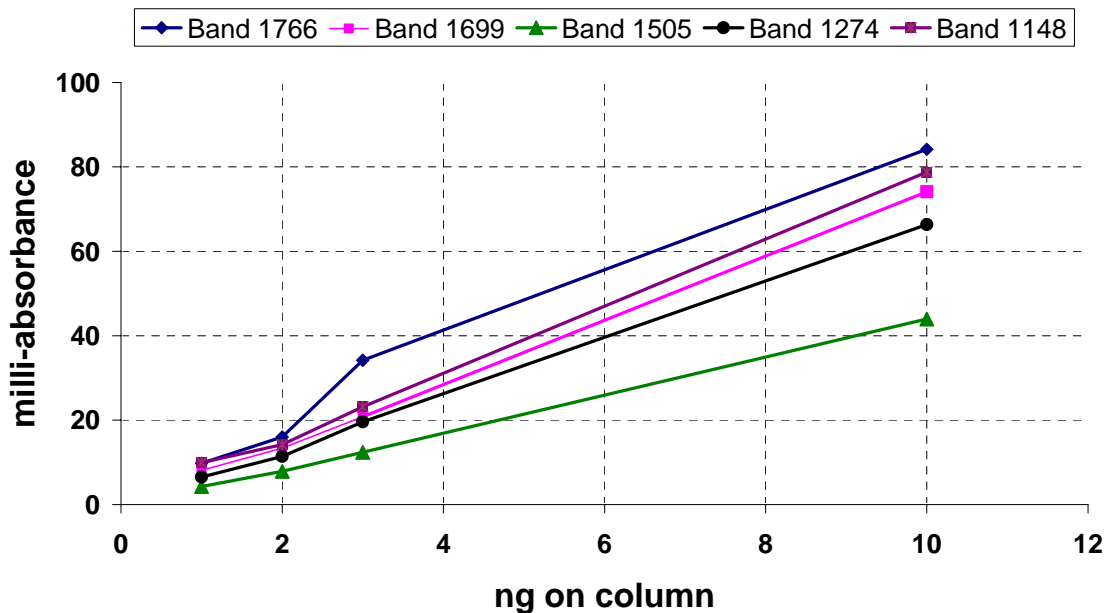
## Vanillin Acetate

Each point is the average of three measurements



## Vanillin Acetate

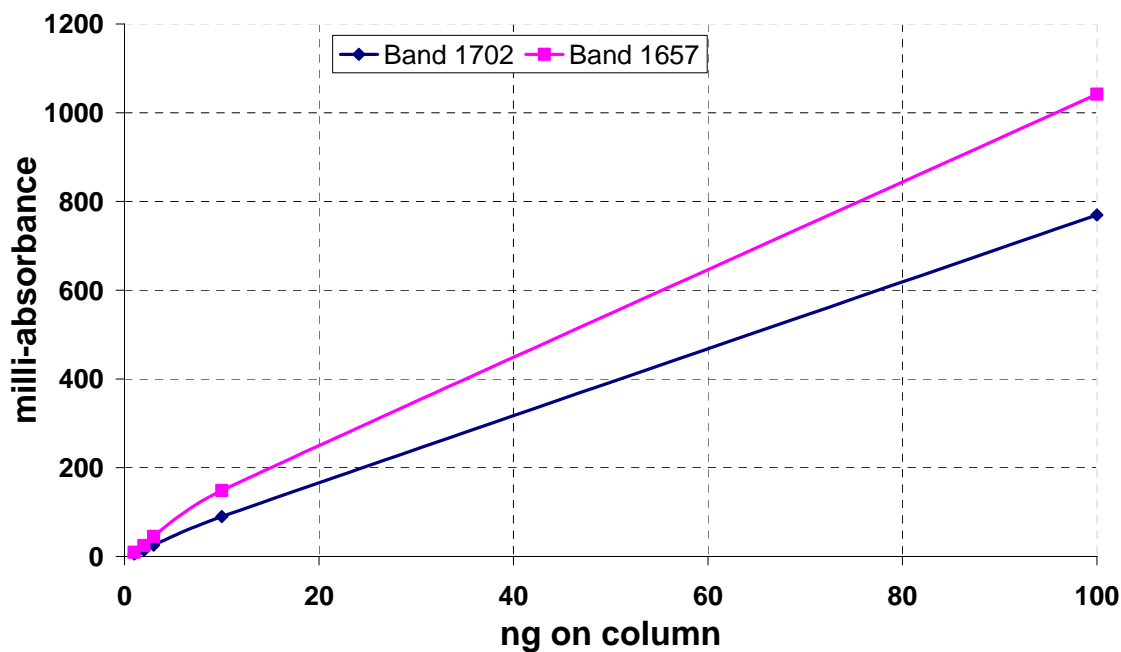
Each point is the average of three measurements





## Caffeine

Each point is average of three measurements



## Caffeine

Each point is average of three measurements

