



3050 Spruce Street  
Saint Louis, Missouri 63103 USA  
Telephone 800-325-5832 • (314) 771-5765  
Fax (314) 286-7828  
email: techserv@sial.com  
sigma-aldrich.com

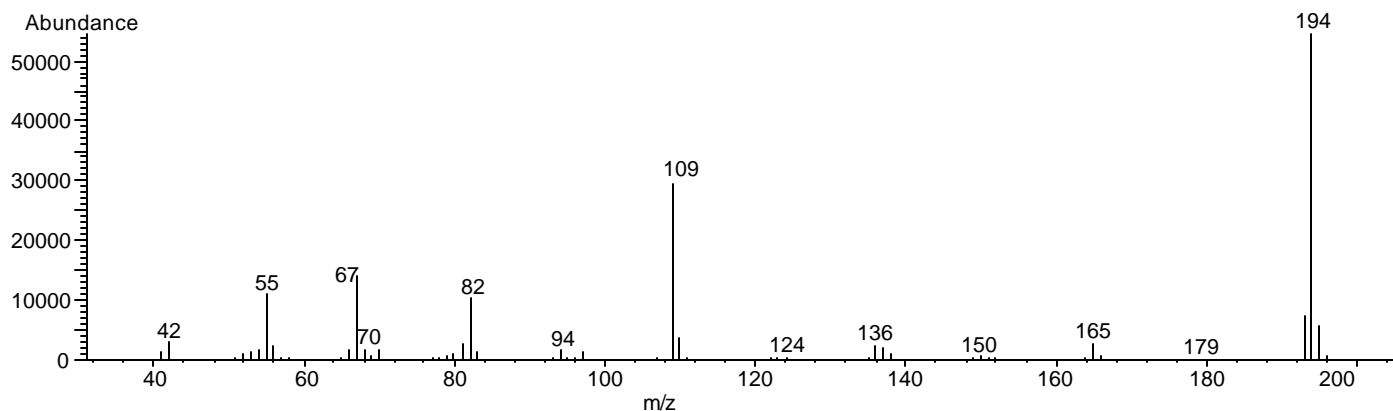
## Product Information

### CAFFEINE

Methanol Solution

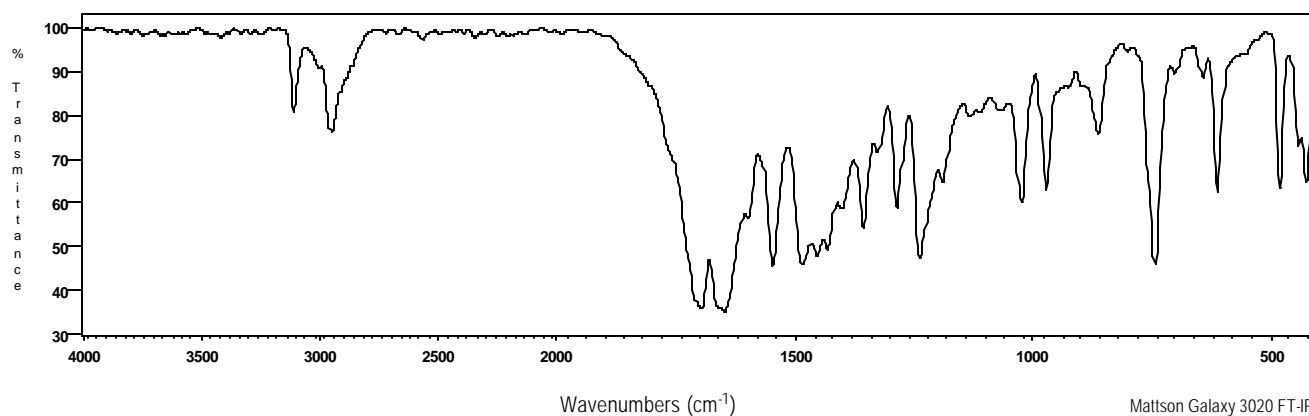
<b>Product Number</b>	C 6035	<b>Synonyms</b>	Coffeinum; Guaranine; Methyltheobromine
<b>Lot Number</b>	015K8803	<b>Stability</b>	If stored at 2-8°C in an air tight container, protected from light, decomposition of the product is less than 1% in 48 months. After opening, concentration may change due to loss of solvent.
<b>CAS Number</b>	[58-08-2]	<b>Expiration Date</b>	December 2008
<b>Concentration</b>	1.00 mg Caffeine/mL GC grade methanol (conc. verified by UV)	<b>Storage</b>	2-8°C.
<b>Molecular Formula</b>	$C_8H_{10}N_4O_2$	<b>DEA Class</b>	Formulation of a non controlled substance
<b>Molecular Weight</b>	194.2		

70 eV Electron Ionization Mass Spectrum



Hewlett-Packard 5890 Series II Gas Chromatograph  
Hewlett-Packard 5971 Mass Selective Detector  
Hewlett-Packard G1034C MS ChemStation (HP-DOS series)

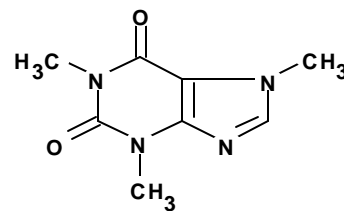
FT-IR



Mattson Galaxy 3020 FT-IR  
KBr Pellet

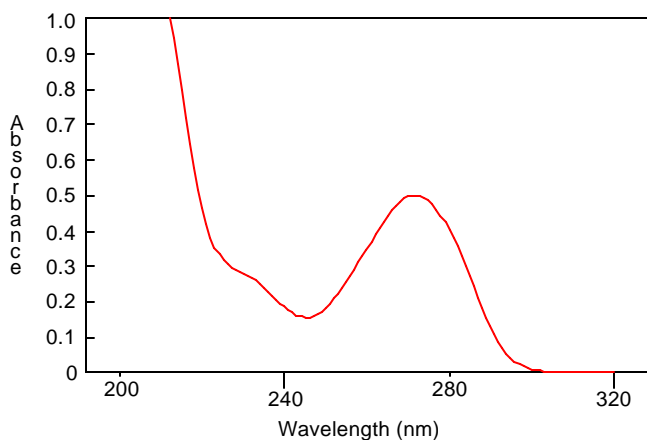
# CAFFEINE

Methanol Solution  
Product Number C 6035  
Lot Number 015K8803



## Ultraviolet Spectrum

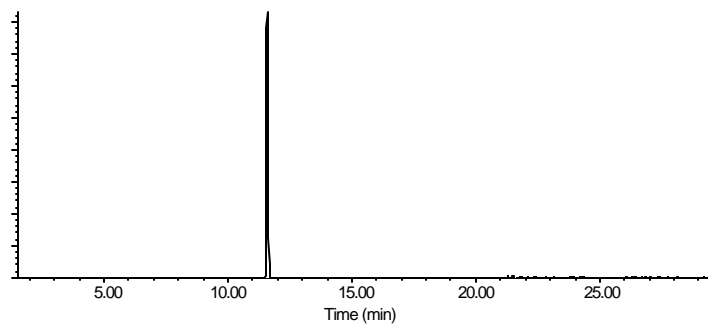
<b>Peak</b>	272.0 nm
<b>Absorbance</b>	0.502
<b>Solvent</b>	0.2 N H <sub>2</sub> SO <sub>4</sub>
<b>Dilution</b>	1:99 (v/v)



Bio-Tek Uvikon XL

## Capillary Gas Chromatography

**Column** Supelco SPB-1 (Cat. No. 2-4162)  
**I.D.** 0.20 mm **Length** 15 m **Film Thickness** 0.20  $\mu$ m  
**Oven Temperature** 50°C (2 min.), then 15°/min. to 300°C, hold 11 min.  
**Injector Temperature** 250°C, Split  
**Detector** Hewlett-Packard 5971  
Mass Selective Detector (70 eV, 40-500 m/z)



Hewlett-Packard 5890

C 6035/015K8803/01/26/05

This product is not for *in vitro* diagnostic procedures. For R&D use only. Not for drug, household or other uses.

Sigma brand products are sold through Sigma-Aldrich, Inc.

Sigma-Aldrich, Inc. warrants that its products conform to the information contained in this and other Sigma-Aldrich publications.

Purchaser must determine the suitability of the product(s) for their particular use. Additional terms and conditions may apply.

Please see reverse side of the invoice or packing slip.