

Conditions

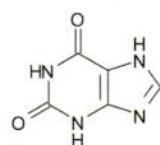
**Column:** ACE Excel 5 SuperC18  
**Dimensions:** 150 x 4.6 mm  
**Part Number:** EXL-1211-1546U  
**Mobile Phase:** A: 20 mM ammonium acetate pH 7.0 in H<sub>2</sub>O  
 B: 20 mM ammonium acetate pH 7.0 in MeCN/H<sub>2</sub>O (90:10 v/v)  
**Gradient:**

Time (mins)	%B
0	2
45	15
48	15
49	2
59	2

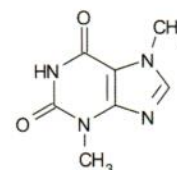
  
**Flow Rate:** 1 mL/min  
**Injection:** 1 µL  
**Temperature:** 60 °C  
**Detection:** UV, 273 nm

Analytes

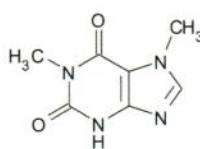
1. Xanthine
2. Theobromine
3. Paraxanthine
4. Theophylline
5. Caffeine



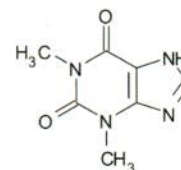
Xanthine



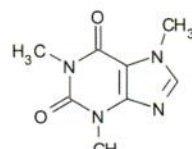
Theobromine



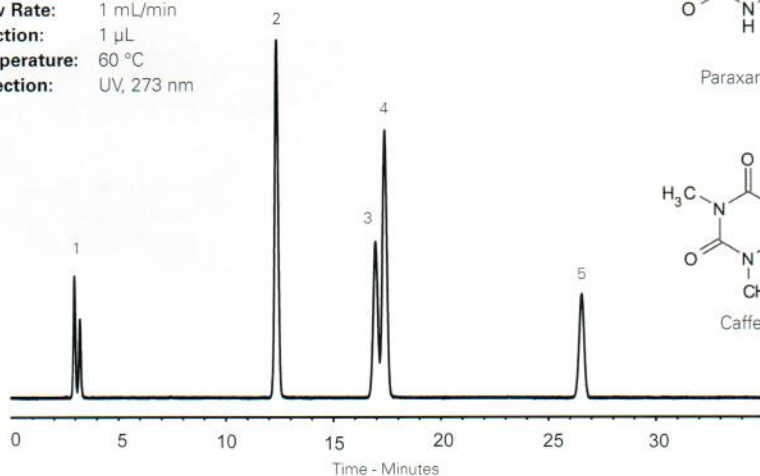
Paraxanthine



Theophylline



Caffeine



Caffeoylquinic and Dicafeoylquinic Acids

Conditions

**Column:** ACE UltraCore 2.5 SuperC18  
**Dimensions:** 100 x 4.6 mm  
**Part Number:** CORE-25A-1046U  
**Mobile Phase:** A: 0.2% phosphoric acid in H<sub>2</sub>O  
 B: MeCN  
**Gradient:**

Time (mins)	%B
0	5
1	5
9	18
14	28
15	70

  
**Flow Rate:** 0.8 mL/min  
**Temperature:** 35 °C  
**Detection:** UV-Vis, 327 nm

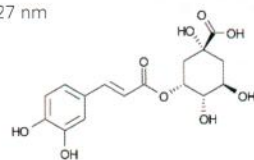
Analytes

1. 3-Caffeoylquinic acid (chlorogenic acid)
2. 5-Caffeoylquinic acid (neochlorogenic acid)
3. 4-Caffeoylquinic acid (cryptochlorogenic acid)
4. Feruloylquinic acid
5. 3,4-Dicafeoylquinic acid (isochlorogenic acid B)
6. 3,5-Dicafeoylquinic acid (isochlorogenic acid A)
7. 4,5-Dicafeoylquinic acid (isochlorogenic acid C)

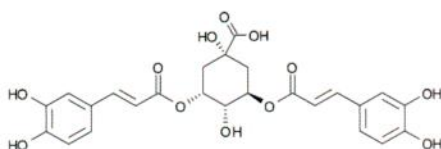
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5-Caffeoylquinic acid (neochlorogenic acid)



3,5-Dicafeoylquinic acid (isochlorogenic acid A)

