Recommended methods for the Identification and Analysis of Cocaine in Seized Materials
3. Description of the pure compounds

The compounds listed below include cocaine, major components (> 1% by weight) and minor components (usually < 1% by weight). Trace components (usually < 0.1% by weight and typically requiring an extraction step) are not described here.

**Cocaine**

![Cocaine structure]

**Synonyms:**
1R-(exo,exo)-3-(Benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid methyl ester
3β-Hydroxy-1αH,5αH-tropane-2β-carboxylic acid methyl ester benzoate
Ecgonine methyl ester benzoate
1-Cocaine
β-Cocaine
Benzoylmethylecgonine

C_{17}H_{21}NO_4
Molecular Weight = 303.4 (base), 339.8 (hydrochloride)
Melting point: 98° C (base), 195° C (hydrochloride)

<table>
<thead>
<tr>
<th>Solubilities (1g/ml):</th>
<th>Base</th>
<th>Hydrochloride</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>slightly soluble (1 in 600)</td>
<td>soluble (1 in 0.4)</td>
</tr>
<tr>
<td>Ethanol</td>
<td>soluble (1 in 6.5)</td>
<td>soluble (1 in 3.2)</td>
</tr>
<tr>
<td>Diethyl ether</td>
<td>soluble (1 in 3.5)</td>
<td>practically insoluble</td>
</tr>
<tr>
<td>Chloroform</td>
<td>soluble (1 in 0.7)</td>
<td>soluble (1 in 12.5)</td>
</tr>
</tbody>
</table>
Recommended Methods for the Identification and Analysis of Cocaine in Seized Materials

**GC-MS data (percentage abundance):**
303 (M⁺, 17), 182 (71), 105 (29), 96 (24), 94 (36), 82 (100), 77 (35) m/z

**NMR data (hydrochloride):**

\[ ^1H \) NMR 600 MHz; (D₂O): δ 2.90 (3H, s), 3.63 (3H, s), 3.65 (1H, dd), 4.10 (1H, bm), 4.24 (1H, bm), 5.59 (1H, ddd), 7.54, (1H, t), 7.70 (1H, t), 7.96 (1H, d) ppm

\[ ^13C \) NMR (151 MHz; D₂O): δ 22.8, 23.9, 32.8, 39.1, 46.3, 53.6, 63.4, 64.1, 64.7, 128.7, 129.2, 129.8, 134.7, 167.5, 173.6 ppm

**Infrared data:**
Principal peaks at wavenumbers 1710, 1738, 1275, 1110, 712, 1037 cm⁻¹ (KBr disk).

**UV Data:**
Aqueous acid—233 nm (A₁ = 430), 275 nm

Major and minor components

*Cinnamoylcocaine*

![Chemical Structure]

**Synonyms:**

- [1R-(exo,exo)]-8-Methyl-3-[(1-oxo-3-phenyl-2-propenyl)oxy]-8-azabicyclo[3.2.1]octane-2-carboxylic acid methyl ester
- Ecgonine cinnamate methyl ester
- Cinnamoylecgtoninmethyl ester
- Cinnamoylmethylecgonine
- Cinnamylcocaine

C₁₉H₂₃NO₄
Molecular Weight: 329.4
Melting point: 121° C (base)
Solubilities (1g/ml): 

<table>
<thead>
<tr>
<th></th>
<th>Base</th>
<th>Hydrochloride</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>almost insoluble</td>
<td>soluble</td>
</tr>
<tr>
<td>Ethanol</td>
<td>soluble</td>
<td>soluble</td>
</tr>
<tr>
<td>Diethyl ether</td>
<td>soluble</td>
<td>soluble</td>
</tr>
<tr>
<td>Chloroform</td>
<td>soluble</td>
<td>slightly</td>
</tr>
</tbody>
</table>

**GC-MS data (percentage abundance):**

329 (M⁺, 15), 238 (14), 182 (72), 131 (33), 103 (24), 96 (59), 94 (35), 82 (100), 42 (27) m/z

**NMR data (hydrochloride):**

1H NMR (300 MHz; CDCl₃): (Key spectral data): δ 2.21 (3H, s), 2.40 (1H, ddd), 3.71 (3H, s), 5.11 (1H, ddd), 6.44 (1H, d), 7.36 (3H, m), 7.51 (2H, m), 7.65 (1H, d) ppm

13C NMR (75.5 MHz; CDCl₃): δ 25.2, 25.4, 35.5, 41.2, 50.1, 51.4, 61.6, 64.8, 66.6, 118.3, 128.1 (x 2), 128.8 (x 2), 130.2, 134.4, 144.9, 166.7, 170.8 ppm

**Infrared data:**

Principal peaks at wavenumbers 2959, 2856, 2804, 1749, 1699, 1630, 1319, 1179, 1037, 1008, 767, 683 cm⁻¹ (KBr disk)

**Methylecgonine**

\[
\begin{align*}
\text{Synonyms:} & \quad [1R-(\text{exo,exo})]-3-\text{Hydroxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid methyl ester} \\
& \quad \text{Ecgonine methyl ester} \\
& \quad 3\beta-\text{Hydroxy-1}H,5\alpha\text{H-tropane-2β-carboxylic acid methyl ester} \\
\end{align*}
\]

C₁₀H₁₇NO₃

Molecular Weight: 199.3 (base), 235.7 (hydrochloride)

Melting point: oil (base), 215° C (hydrochloride)
GC-MS data (percentage abundance):
199 (M+, 30), 168 (18), 112 (12), 96 (78), 94 (38), 82 (100), 68 (8), 42 (32) m/z

NMR data (hydrochloride):

$^1$H NMR (500 MHz; D$_2$O): $\delta$ 2.03-2.14 (3H, m), 2.20-2.24 (1H, m), 2.30-2.48 (2H, m), 2.83 (3H, s), 3.31 (1H, dd, $J = 2.2, 7.2$ Hz), 3.80 (3H, s) 3.99 (1H, m), 4.15 (1H, bd, $J = 7.0$ Hz), 4.43-4.48 (1H, m) ppm

$^{13}$C NMR (125 MHz; D$_2$O): $\delta$ 22.5, 23.5, 34.8, 38.4, 48.8, 52.8, 60.3, 63.1, 63.8, 174.2 ppm

Infrared data:
Principal peaks at wavenumbers 3269, 2963, 2132, 1704, 1481, 1428, 1350, 1215, 1140, 1049, 1013, 968, 777, 616 cm$^{-1}$ (KBr disk).

**Benzoylecgonine**

[Chemical structure image]

**Synonyms:** 3-(Benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid
3β-Hydroxy-1αH,5αH-tropane-2β-carboxylic acid benzoate
Ecgonine benzoate

$C_{16}H_{19}NO_4$
Molecular Weight: 289.3
Melting point: 195° C (anhydrous) (decomposes), 86-92° C (tetrahydrate), 200° C hydrochloride

<table>
<thead>
<tr>
<th>Solubilities (1g/ml):</th>
<th>Base</th>
<th>Hydrochloride</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water, boiling</td>
<td>soluble</td>
<td>soluble</td>
</tr>
<tr>
<td>Ethanol</td>
<td>soluble</td>
<td>soluble</td>
</tr>
</tbody>
</table>

GC-MS data (percentage abundance):
289 (M+, 5), 168 (26), 124 (100), 105 (31), 96 (19), 94 (26), 82 (61), 77 (40), 67 (11) m/z
**NMR data (hydrochloride):**

$^1$H NMR (300 MHz; D$_2$O): (Key spectral data): δ 2.61-2.17 (6H, m) 2.88 (3H, s), 3.22 (1H, dd), 4.07 (2H, bd), 5.54 (1H, m), 7.59 (2H, dd), 7.76 (1H, dd), 8.06 (2H, d) ppm

$^{13}$C NMR (75.5 MHz; D$_2$O): δ 23.2, 32.6, 37.6, 48.8, 62.3, 64.8, 128.7, 128.9, 129.5, 133.9, 167.2, 176.9 ppm

**Infrared data:**
Principal peaks at wavenumbers 1275, 1720, 1618, 717, 1116, 1316 cm$^{-1}$

**UV Data:**
Aqueous acid—234 nm (A$\lambda$ = 376), 274 nm

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**Ecgonine**

![Ecgonine structure](image)

**Synonyms:**
- [1R-(exo,exo)]-3-Hydroxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid
- 3β-Hydroxy-1αH,5αH-tropane-2β-carboxylic acid

C$_9$H$_{15}$NO$_3$

Molecular Weight: 185.2 (base), 221.7 (hydrochloride)

Melting point: 198° C (base), 246° C (hydrochloride)

**Solubilities (1g/ml):**

<table>
<thead>
<tr>
<th></th>
<th>Base</th>
<th>Hydrochloride</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>soluble</td>
<td>soluble</td>
</tr>
<tr>
<td>Ethanol</td>
<td>slightly soluble</td>
<td>slightly soluble</td>
</tr>
<tr>
<td>Diethyl ether</td>
<td>sparingly soluble</td>
<td></td>
</tr>
<tr>
<td>Chloroform</td>
<td>sparingly soluble</td>
<td></td>
</tr>
</tbody>
</table>

**GC-MS data (percentage abundance):**
185 (M$^+$, 9), 124 (33), 96 (82), 82 (100), 57 (54), 42 (89) m/z
**Recommended Methods for the Identification and Analysis of Cocaine in Seized Materials**

**NMR data (hydrochloride):**

$^1$H NMR (600 MHz; D$_2$O): δ 1.98-2.19 (4H, m), 2.25-2.41 (2H, m), 2.78 (3H, s), 3.18 (1H, dd, $J = 2.3, 7.1$ Hz), 3.92 (1H, m), 4.10 (1H, d, $J = 7.3$ Hz), 4.41 (1H, m) ppm

$^{13}$C NMR (150 MHz; D$_2$O): δ 23.2, 24.0, 35.5, 38.9, 49.5, 60.8, 63.6, 64.6, 176.4 ppm

**Infrared data:**

Principle peaks at wavenumbers 1688, 1210, 1200, 1223, 1134, 1179 cm$^{-1}$ (ecgonine hydrochloride, KBr disk)

**UV Data:**

Ethanol—275 nm

**Norcocaine**

![Norcocaine structure](image)

**Synonyms:** 1R-(exo,exo)-3-(Benzoyloxy)-8-azabicyclo[3.2.1]octane-2-carboxylic acid methyl ester

C$_{16}$H$_{19}$NO$_4$

Molecular Weight: 289.3 (base), 325.8 (hydrochloride)

Melting point: 115-116° C (hydrochloride)

**Solubilities (1g/ml):**

<table>
<thead>
<tr>
<th>Solubility (1g/ml)</th>
<th>Hydrochloride</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>soluble</td>
</tr>
<tr>
<td>Ethanol</td>
<td>slightly soluble</td>
</tr>
</tbody>
</table>

**GC-MS data (percentage abundance):**

289 (M$^+$, 11), 168 (100), 136 (37), 108 (25), 105 (23), 82 (13), 80 (23), 77 (33), 68 (41) m/z
NMR data (hydrochloride):

$^1$H NMR (500 MHz; D$_2$O): (Key spectral data): $\delta$ 3.59 (1H, dd), 3.64 (3H, s), 4.38 (1H, bd), 5.56 (1H, ddd), 7.54 (2H, t), 7.71 (1H, t), 7.95 (1H, d) ppm

$^{13}$C NMR (75.5 MHz; CDCl$_3$): $\delta$ 24.4, 25.1, 31.1, 44.9, 53.0, 54.3, 55.4, 65.0, 128.4, 128.8, 129.4, 134.3, 167.0, 173.0 ppm

Infrared data:

Principle peaks at wavenumbers 3597, 3408, 3152, 2951, 2772, 2744, 2527, 1721, 1440, 1350, 1275, 717 cm$^{-1}$

Cinnamic acid (trans-)

![Cinnamic acid structure]

Synonyms: 3-phenyl-2-propenoic acid
$\beta$-phenylacrylic acid

C$_{9}$H$_{8}$O$_{2}$

Molecular Weight: 148.2

Melting point: 133° C (base)

<table>
<thead>
<tr>
<th>Solubilities (1g/ml)</th>
<th>Base</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>slightly soluble</td>
</tr>
<tr>
<td>Ethanol</td>
<td>soluble</td>
</tr>
<tr>
<td>Diethyl ether</td>
<td>soluble</td>
</tr>
<tr>
<td>Chloroform</td>
<td>soluble</td>
</tr>
</tbody>
</table>

GC-MS data (percentage abundance):

148 (M$^+$, 74), 148 (100), 147 (100), 131 (22), 103 (61), 77 (47), 51 (40) m/z

UV Data:

Ethanol—273 nm
**N-Formylnorcocaine**

![Chemical structure of N-Formylnorcocaine](image)

**Synonyms:** [1R-\((exo,exo)\)-3-\((\text{Benzoxyloxy})\)-8-formyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid methyl ester]

\[\text{C}_{17}\text{H}_{19}\text{NO}_{5}\]

**Molecular Weight:** 317.3

**GC-MS data (percentage abundance):**

- 289 (38), 195 (39), 168 (100), 136 (42), 105 (94), 77 (58), 68 (48) m/z.

**NMR data:**

\(^1\)H NMR (600 MHz; CDCl\(_3\)): Double resonances observed due to restricted rotation about the amide bond. Rotamers present in ca. 1:1 ratio at room temperature. Key spectral data:

- **Rotamer A** \(\delta \) 2.37 (1H, ddd), 3.25 (1H, bdd, \(s\)), 3.65 (3H, \(s\)), 4.30 (1H, bd), 4.81 (1H, m), 5.53 (1H, ddd, \(s\)), 8.02 (0.5H, \(s\)) ppm

- **Rotamer B** \(\delta \) 2.53 (1H, ddd), 3.17 (1H, bdd), 3.68 (3H, \(s\)), 4.27 (1H, m), 4.95 (1H, bd), 5.49 (1H, ddd), 8.16 (1H, \(s\)) ppm

\(^{13}\)C NMR (CDCl\(_3\)): \(\delta \) 26.9, 27.4, 27.9, 28.4, 33.4, 35.4, 48.5, 48.7, 49.3, 51.1, 51.9, 52.0, 53.6, 55.5, 66.2, 66.3, 128.4, 129.6, 129.7, 133.3, 157.8, 158.0, 165.6, 165.7, 169.6, 170.0 ppm

For additional details related to the substances, the reader is referred to the *Multilingual Dictionary of Narcotic Drugs and Psychotropic Substances Under International Control* (http://www.unodc.org/unodc/en/scientists/multilingual-dictionary-of-narcotic-drugs-and-psychotropic-substances-under-international-control.html), the widely used Merck Index [1] and *Clarke's Analysis of Drugs and Poisons* [2].