Udes09 hydrochloride

The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material.

![Chemical Structure](image)

1. GENERAL INFORMATION

**IUPAC Name:** N-((1R,2R)-2-(dimethylamino)cyclohexyl)-2-chloronicotinamide; hydrochloride

**CAS#:** N/A

**Synonyms:** Udes09

**Source:** Synthesized Material Lot# JLK010-054-Udes09

**Appearance:** light brown solid (HCl)

**UV$_{max}$ (nm):** Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

<table>
<thead>
<tr>
<th>Form</th>
<th>Chemical Formula</th>
<th>Molecular Weight</th>
<th>Melting Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCl</td>
<td>C$<em>{14}$H$</em>{20}$ClN$_3$O-HCl</td>
<td>318.24</td>
<td>123.2 ± 2.81</td>
</tr>
<tr>
<td>Base</td>
<td>C$<em>{14}$H$</em>{20}$ClN$_3$O</td>
<td>281.78</td>
<td>Not determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated chloroform:methanol (CDCl₃:CD₃OD, 1:5) + TMS.

Instrument: 400 MHz NMR spectrometer
Parameters: Spectral width: 6410.3 Hz containing -3 ppm through 13 ppm
Pulse angle: 90°
Delay between pulses: 30 seconds

¹H NMR: Udes09 HCl; Lot JLK010-054-Udes09; CDCl₃:CD₃OD (1:5) + TMS; 400 MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~ 1 mg/mL in methanol

Instrument: Shimadzu gas chromatograph operated in split mode with MS detector

Column: Rtx5MS (a DB-5 equivalent); 30m x 0.25 mm x 0.25 µm

Carrier Gas: Helium at 1 mL/min

Temperatures: Injector: 280°C

MSD transfer line: 280°C

MS Source: 200°C

Oven program:
1) 90°C initial temperature for 2.0 min
2) Ramp to 300°C at 14°C/min
3) Hold final temperature for 10.0 min

Injection Parameters: Split Ratio = 1:15, 1 µL injected

MS Parameters:
Mass scan range: 34-550 amu
Threshold: 100
Tune file: 050218_Tune.qgt
Acquisition mode: scan

Retention Time: 14.72 min

EI Mass Spectrum: Udes09 HCl; Lot JLK010-054-Udes09

Chemical Formula: C14H21ClN3O+
Exact Mass: 282.13677
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Zoomed view (84.10 and 125.15 are truncated in this view)
Udes09 hydrochloride

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3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)
Scan Parameters:
- Number of scans: 4
- Number of background scans: 4
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 8
- Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): Udes09 HCl; Lot JLK010-054-Udes09
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3.4 RAMAN SPECTROSCOPY

Instrument: Rigaku Progeny 1064
Scan Parameters:
- Power (mW): 350
- Exposure (ms): 1000
- Averages: 30
- Threshold: 0.80

Raman (1064 nm): Udes09 HCl; Lot JLK010-054-Udes09
4. ADDITIONAL RESOURCES

ANALGESIC N-(2-AMINO CYCLOALIPHATIC) BENZAMIDES
Szmuszkovicz

Benzeneacetamide amines: structurally novel non-mu opioids
J. Szmuszkovicz, and P.F. Von Voigtlander
Journal of Medicinal Chemistry 1982, 25 (10), 1125–1126
DOI: 10.1021/jm00352a005

Factors affecting binding of trans-N-[2-(methylamino)cyclohexyl]benzamides at the primary morphine receptor
B.V. Cheney, J. Szmuszkovicz, R.A. Lahti and D.A. Zichi
Journal of Medicinal Chemistry 1985, 28 (12), 1853–1864
DOI: 10.1021/jm00150a017

Single stereoisomer analogs in the U-47700 series:

5. ACKNOWLEDGEMENT

These data are from a project supported by Award No. 2016-R2-CX-0059, awarded by the National Institute of Justice, Office of Justice Programs, U.S. Department of Justice. The opinions, findings, and conclusions or recommendations expressed in this publication are those of the authors and do not necessarily reflect those of the Department of Justice. We also thank Rigaku Corporation for the loan of the Progeny 1064 Raman instrument.