1. GENERAL INFORMATION

**IUPAC Name:** 1-(4-trifluoromethylbenzamidomethyl)-cyclohexylidimethylamine; hydrochloride

**CAS#:** 940753-21-9 (base)

**Synonyms:** A04

**Source:** Synthesized Material Lot# JLK008-041-04

**Appearance:** Light Brown Crystals (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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HCl</td>
<td>C$<em>{17}$H$</em>{23}$F$<em>{3}$N$</em>{2}$O·HCl</td>
<td>364.83</td>
<td>231.2 ± 1.56</td>
</tr>
<tr>
<td>base</td>
<td>C$<em>{17}$H$</em>{23}$F$<em>{3}$N$</em>{2}$O</td>
<td>328.37</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 (CDCl₃) + 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: A04 HCl; Lot JLK008-041-04; CDCl₃+ TMS; 400 MHz

![NMR spectrum diagram]
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:** 14.31 min
A04 hydrochloride
The Krstenansky lab at the KGI School of Pharmacy and Health Sciences generated this monograph using synthesized material

EI Mass Spectrum: A04 HCl; Lot JLK008-041-04

Chemical Formula: C\textsubscript{17}H\textsubscript{24}F\textsubscript{3}N\textsubscript{2}O\textsuperscript{+}
Exact Mass: 329.18352

Zoomed view (126.2 is 100% relative intensity and is truncated in this view)
A04 hydrochloride

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

3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with ZnSe ATR attachment (1 bounce)
Scan Parameters: Number of scans: 4

Latest Revision: 09/26/2019

SWGDRUG.org/monographs.htm
A04 hydrochloride

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

Number of background scans: 4
Resolution: 4 cm\(^{-1}\)
Sample gain: 8
Aperture: 150

FTIR ATR (ZnSe, 1 Bounce): A04 HCl; Lot JLK008-041-04
A04 hydrochloride

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

%Transmittance vs. Wavenumber (cm⁻¹)
3.4 RAMAN SPECTROSCOPY

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

Raman (1064 nm): A04 HCl; Lot JLK008-041-04
4. ADDITIONAL RESOURCES

1-(3,4-DICHLOROBENZAMIDOMETHYL)CYCLOHEXYLDIMETHYLAMINE
Norman James Harper and George Bryan Austin Veitch

1-(3,4-Dichlorobenzamidomethyl)cyclohexyldimethylamine and related compounds as potential analgesics
N. J. Harper, G. B. A. Veitch, and D. G. Wibberley
Journal of Medicinal Chemistry 1974 17 (11), 1188-1193
DOI: 10.1021/jm00257a012

Tom Hsu, Jayapal Reddy Mallareddy, Kayla Yoshida, Vincent Bustamante, Tim Lee, John L. Krstenansky,
Alexander C. Zambon, Synthesis and pharmacological characterization of ethylenediamine synthetic opioids
in human μ-opiate receptor 1 (OPRM1) expressing cells. Pharmacol. Research & Perspectives 7: e00511

5. ACKNOWLEDGEMENT

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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.