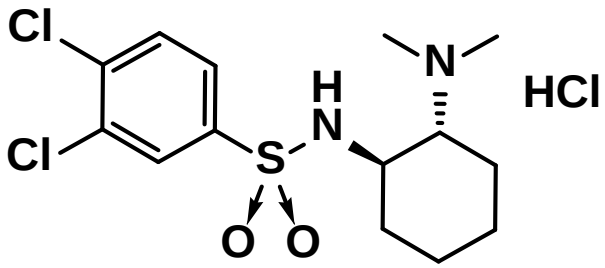
# Udes07 hydrochloride

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




## *1. GENERAL INFORMATION*

***IUPAC Name:*** N-((*1R,2R*)-2-(dimethylamino)cyclohexyl)-3,4-dichlorobenzsulfonamide; hydrochloride

***CAS#:*** N/A

***Synonyms:*** Udes07

***Source:*** **Synthesized Material** Lot# JLK010-054-Udes07

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

***$UV_{max}$ (nm):*** Not Determined

## *2. CHEMICAL AND PHYSICAL DATA*

### 2.1 CHEMICAL DATA

| Form | Chemical Formula | Molecular Weight | Melting Point ($^{o}$C) |
|---|---|---|---|
| HCl | $C_{14}H_{20}Cl_2N_2O_2S{\cdot}HCl$ | 387.74 | 131.1 $\pm$ 2.20 |
| Base | $C_{14}H_{20}Cl_2N_2O_2S$ | 351.29 | Not determined |

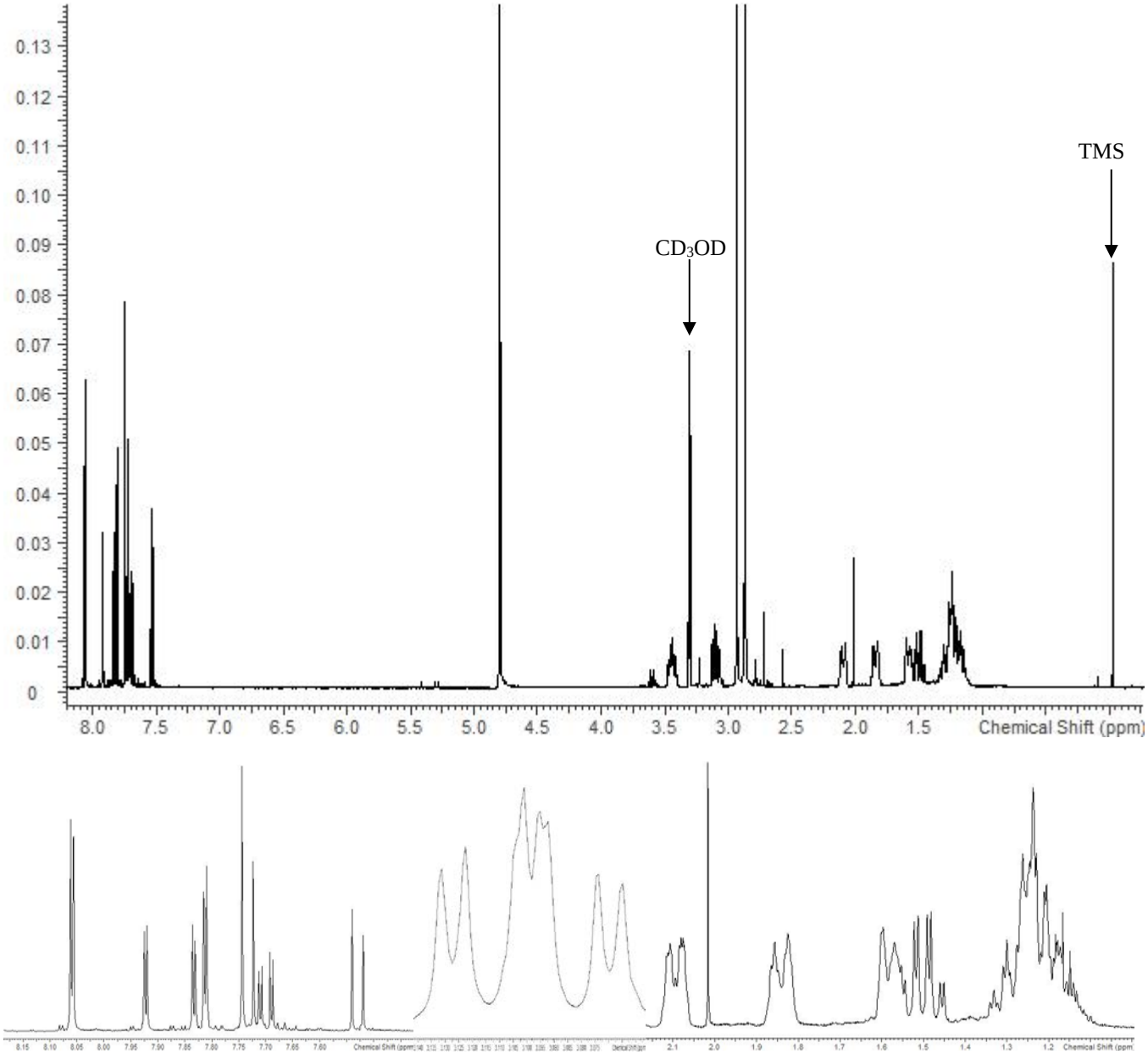
## *3. QUALITATIVE DATA*

### 3.1 NUCLEAR MAGNETIC RESONANCE

*Sample Preparation:* Dilute analyte to ~5 mg/mL in deuterated chloroform:methanol ($CDCl_3$:$CD_3OD$, 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

$^1$H NMR: Udes07 HCl; Lot JLK010-054-Udes07; $CDCl_3$:$CD_3OD$ (1:5) + TMS; 400 MHz

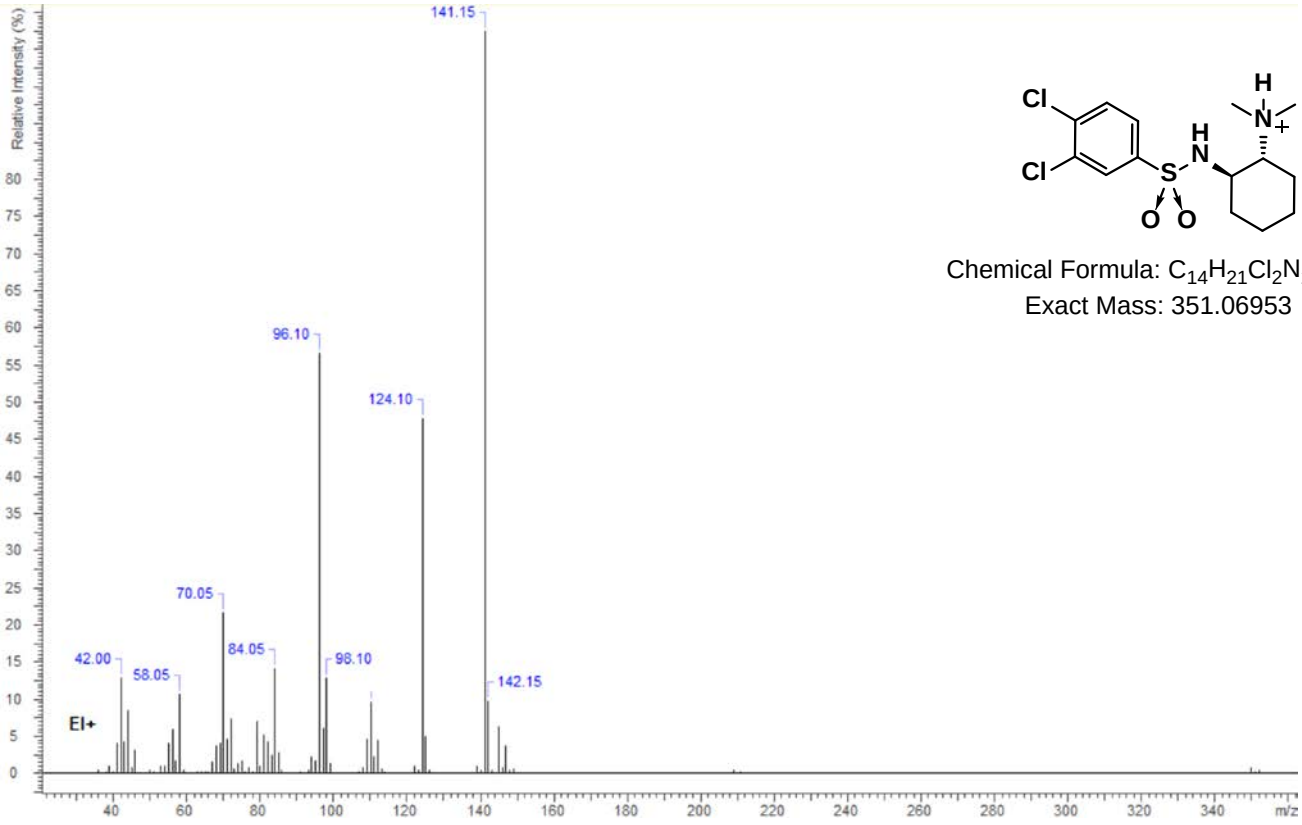


## 3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

*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<br>MSD transfer line: 280°C<br>MS Source: 200°C<br>Oven program:<br>1) 90°C initial temperature for 2.0 min<br>2) Ramp to 300°C at 14°C/min<br>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<br>Threshold: 100<br>Tune file: 050218_Tune.qgt<br>Acquisition mode: scan |
| ***Retention Time:*** | 16.53 min |

EI Mass Spectrum: Udes07 HCl; Lot JLK010-054-Udes07

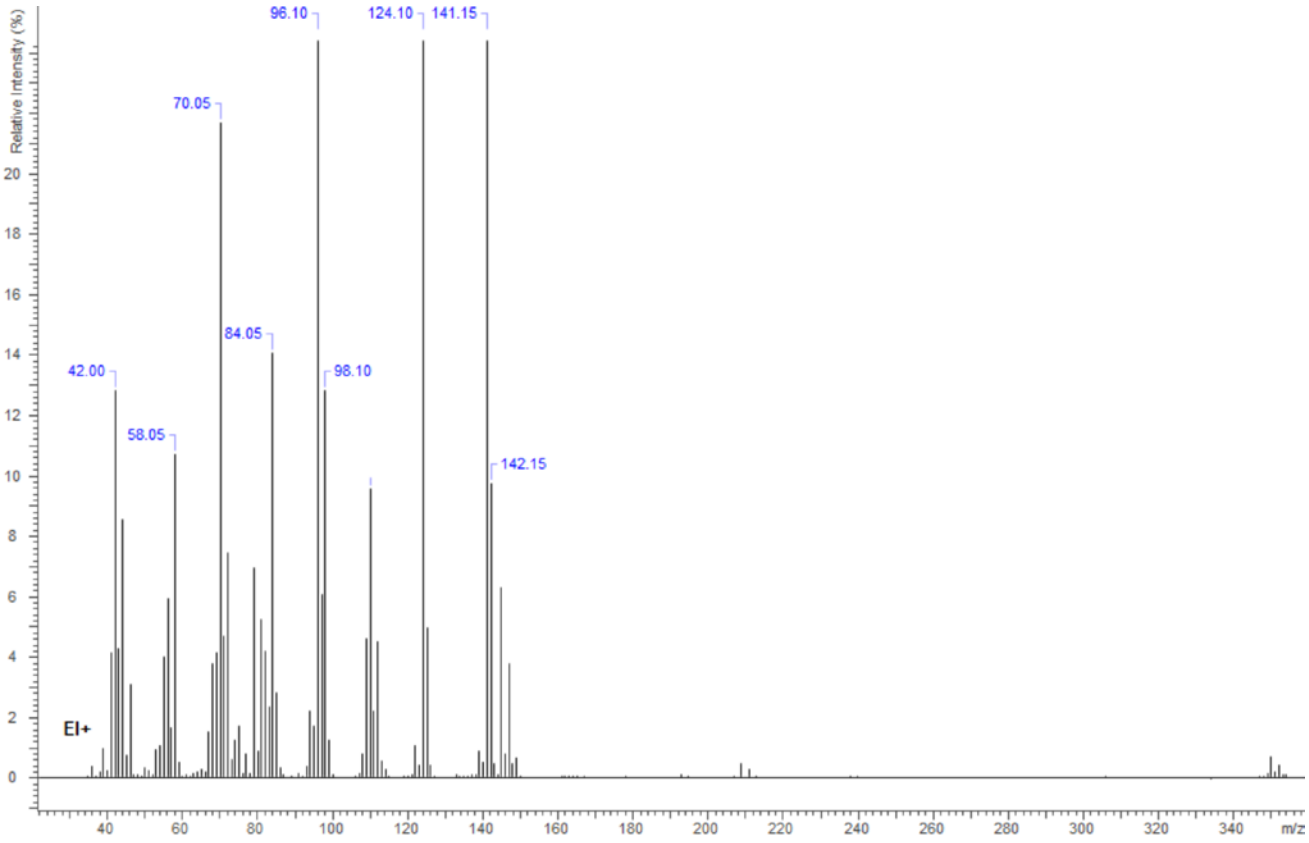






Chemical Formula: $C_{14}H_{21}Cl_2N_2O_2S^+$
Exact Mass: 351.06953

Zoomed view (96.10, 124.10, and 141.15 are truncated in this view)

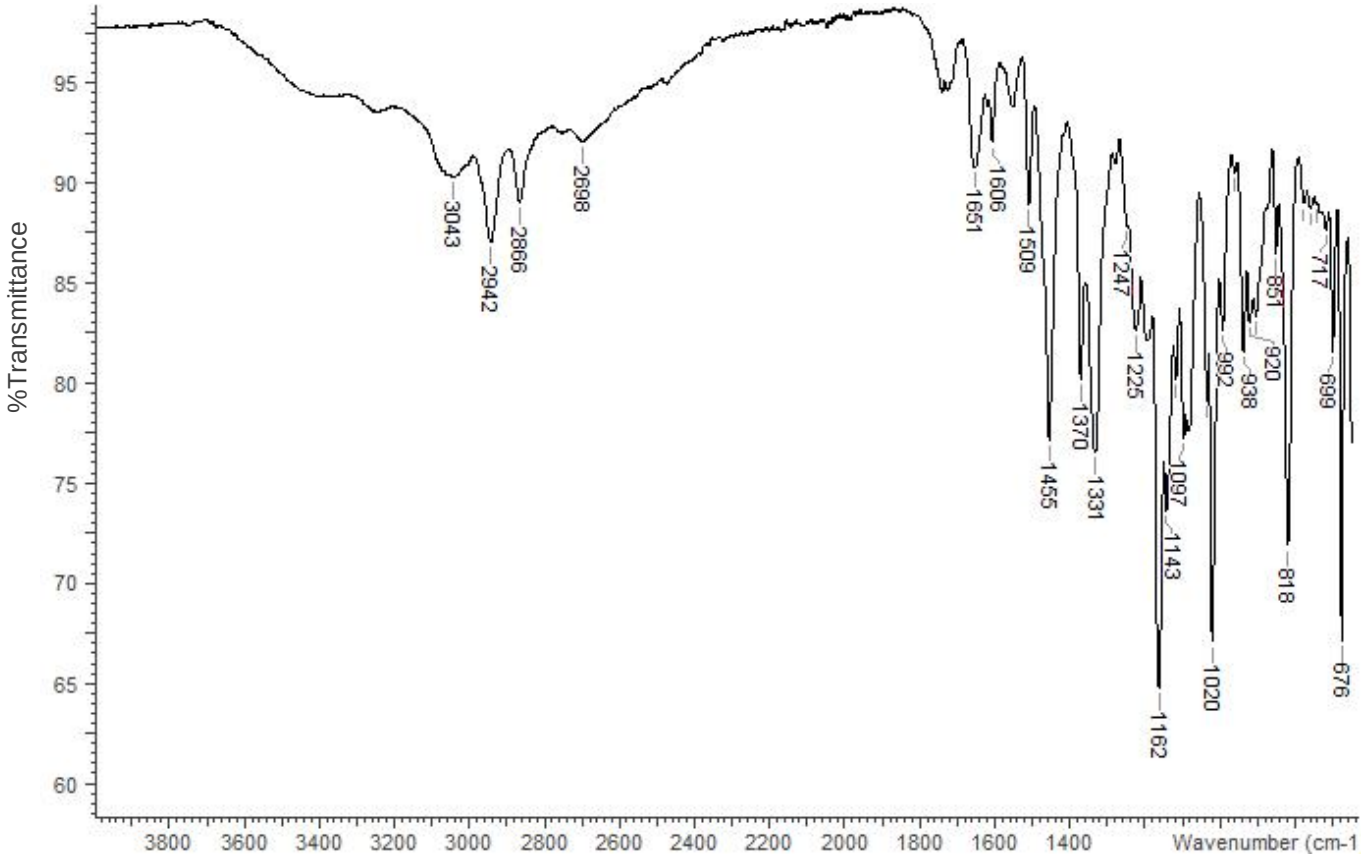


## 3.3 INFRARED SPECTROSCOPY (FTIR)

**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): Udes07 HCl; Lot JLK010-054-Udes07



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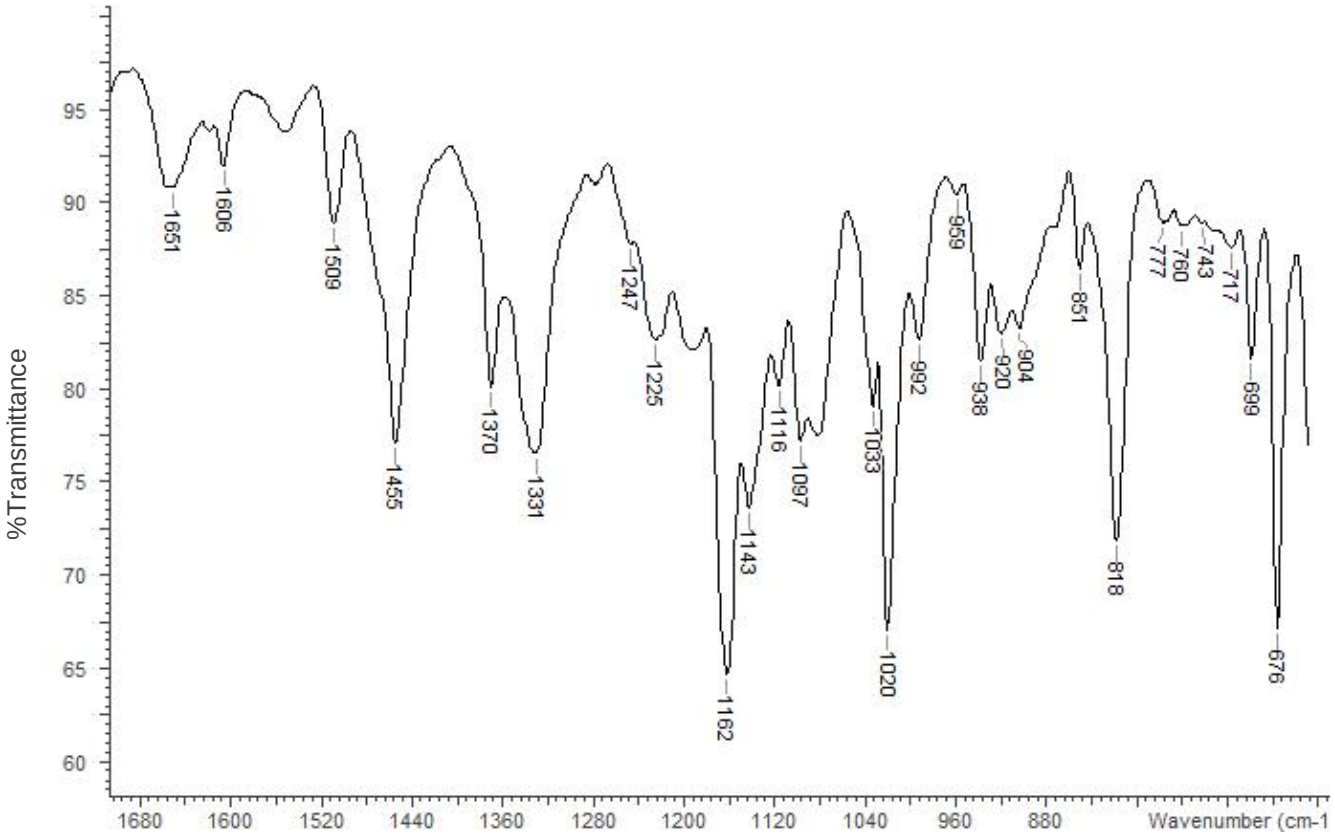

## 4 *ADDITIONAL RESOURCES*

ANALGESIC N-(2-AMINOCYCLOALIPHATIC)BENZAMIDES
Szmuszkovicz
US Patent 4,098, 904 Jul. 4, 1978

Benzeneacetamide amines: structurally novel non-mμ 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:
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 (2019) doi: 10.1002/prp2.511

## 5 *ACKNOWLEDGEMENT*

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