

### 1. GENERAL INFORMATION

**IUPAC Name:** 3-(3-ethylphenyl)-2-methylquinazolin-4(3H)-one

**CFR:** Not Scheduled (9/2013)

**CAS#:** Not Available

**Synonyms:** N/A

**Source:** DEA Reference Material Collection

**Appearance:** White powder (HCl)

**Kovat's Index:** Pending

**UV<sub>max</sub> (nm):** Not Determined

### 2. CHEMICAL AND PHYSICAL DATA

#### 2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O	264	Not Determined
HCl	C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O · HCl	300	236.4

### 3. ADDITIONAL RESOURCES

No resources identified as of 9/2013.

## 4. QUALITATIVE DATA

### 4.1 NUCLEAR MAGNETIC RESONANCE

#### Method NMR $\text{CDCl}_3$

*Sample Preparation:* Dilute analyte to ~10 mg/mL in  $\text{CDCl}_3$  containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

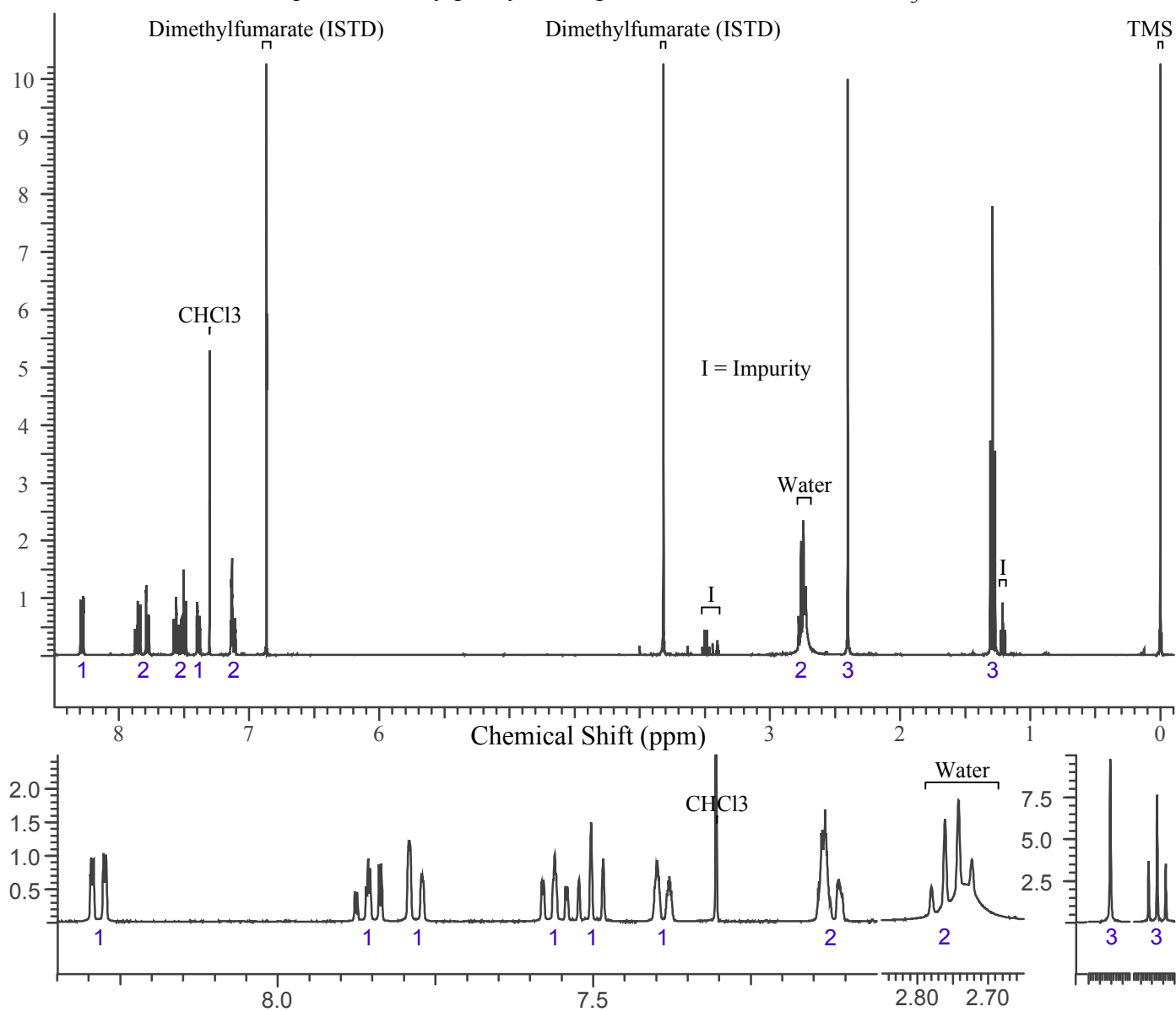
*Instrument:* 400 MHz NMR spectrometer

*Parameters:* Spectral width: at least containing -3 ppm through 13 ppm

Pulse angle:  $90^\circ$

Delay between pulses: 45 seconds

$^1\text{H}$  NMR: Etaqualone 3-ethylphenyl analog HCl; Lot N17-P60A;  $\text{CDCl}_3$ ; 400 MHz



## 4.2 Gas Chromatography/Mass Spectrometry

*Sample Preparation:* Dilute analyte ~ 1 mg/mL in chloroform

***Instrument:*** Agilent gas chromatograph operated in split mode with MS detector

***Column:*** DB-1 MS (or equivalent); 30m x 0.25 mm x 0.25  $\mu$ m

***Carrier Gas:*** Helium at 1 mL/min

***Temperatures:*** Injector: 280°C

MSD transfer line: 280°C

MS Source: 230°C

MS Quad: 150°C

Oven program:

1) 100°C initial temperature for 1.0 min

2) Ramp to 300°C at 12 °C/min

3) Hold final temperature for 9.0 min

***Injection Parameters:*** Split Ratio = 20:1, 1  $\mu$ L injected

***MS Parameters:*** Mass scan range: 30-550 amu

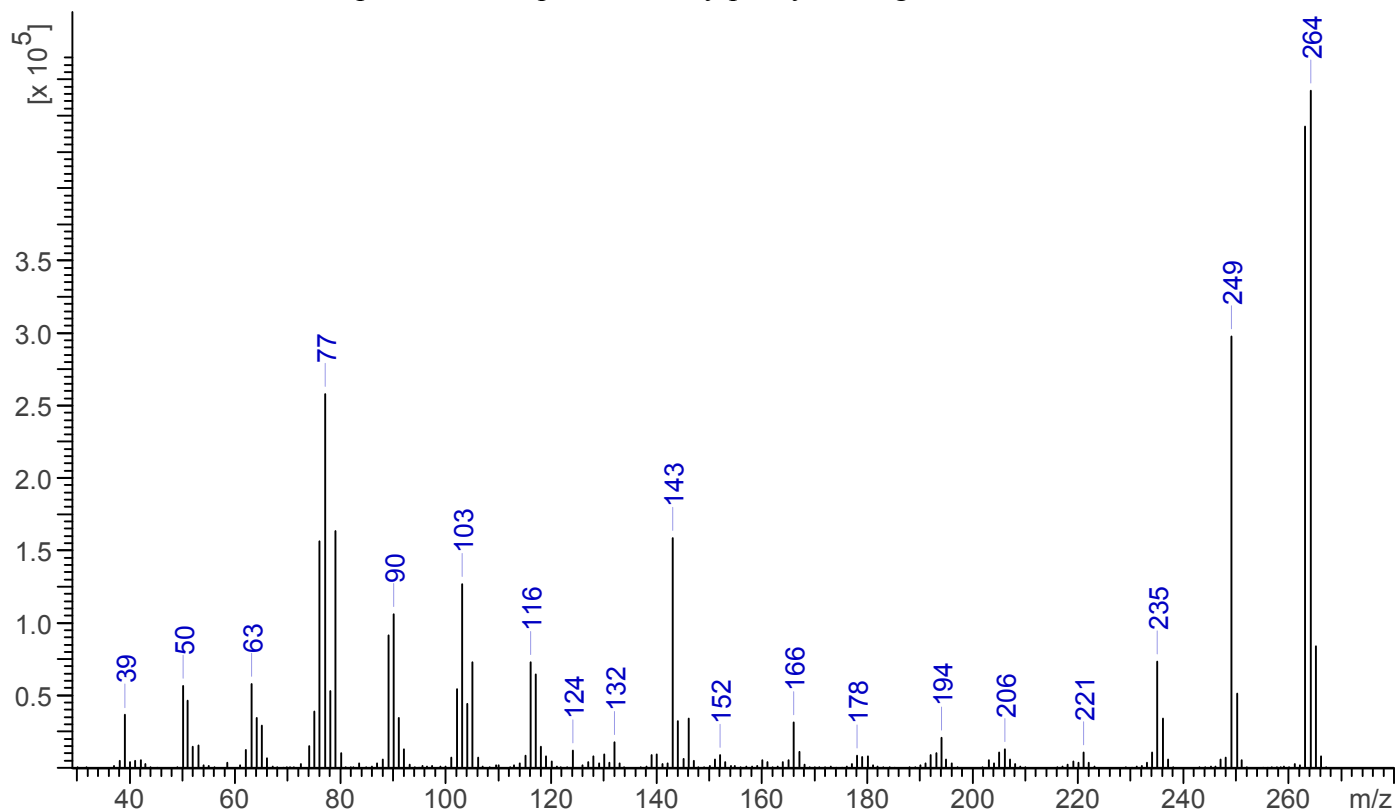
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

***Retention Time:*** 14.677 min

EI Mass Spectrum: Etaqualone 3-ethylphenyl analog HCl; Lot N17-P60A



### 4.3 INFRARED SPECTROSCOPY (FTIR)

**Instrument:** FTIR with diamond ATR attachment (3 bounce)

**Scan Parameters:** Number of scans: 32  
Number of background scans: 32  
Resolution: 4 cm<sup>-1</sup>  
Sample gain: 8  
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): Etaqualone 3-ethylphenyl analog HCl; Lot N17-P60A

