

1. GENERAL INFORMATION

IUPAC Name:	6-methyl-2-[(4-methylphenyl)amino]-4H-3,1-benzoxazin-4-one
CFR:	Not Scheduled (9/2013)
CAS#:	86672-58-4
Synonyms:	None
Source:	DEA Reference Material Collection
Appearance:	Long white crystals
Kovat's Index:	Pending
UV_{max} (nm):	220.0, 246.2, 281.9, 350.6

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	C ₁₆ H ₁₄ N ₂ O ₂	266	Not Determined

3. ADDITIONAL RESOURCES

Tarzia, G., Antonietti, F., Duranti, A., Tontini, A., Mor, M., Rivara, S., Traldi, P., Astarita, G., King, A., Clapper, J.R., Piomelli, D. Identification of a bioactive impurity in a commercial sample of 6-methyl-2-*p*-tolylaminobenzo[d][1,3]oxazin-4-one (URB754). *Annali di Chimica* **2007**, 97, 887-894.

[Forendex](#)

[Wikipedia](#)

4. QUALITATIVE DATA

4.1 NUCLEAR MAGNETIC RESONANCE

Method NMR DMSO

Sample Preparation: Dilute analyte to ~5 mg/mL in deuterated dimethyl sulfoxide (DMSO-*d*₆) containing TMS for 0 ppm reference and dimethylfumarate as quantitative internal standard.

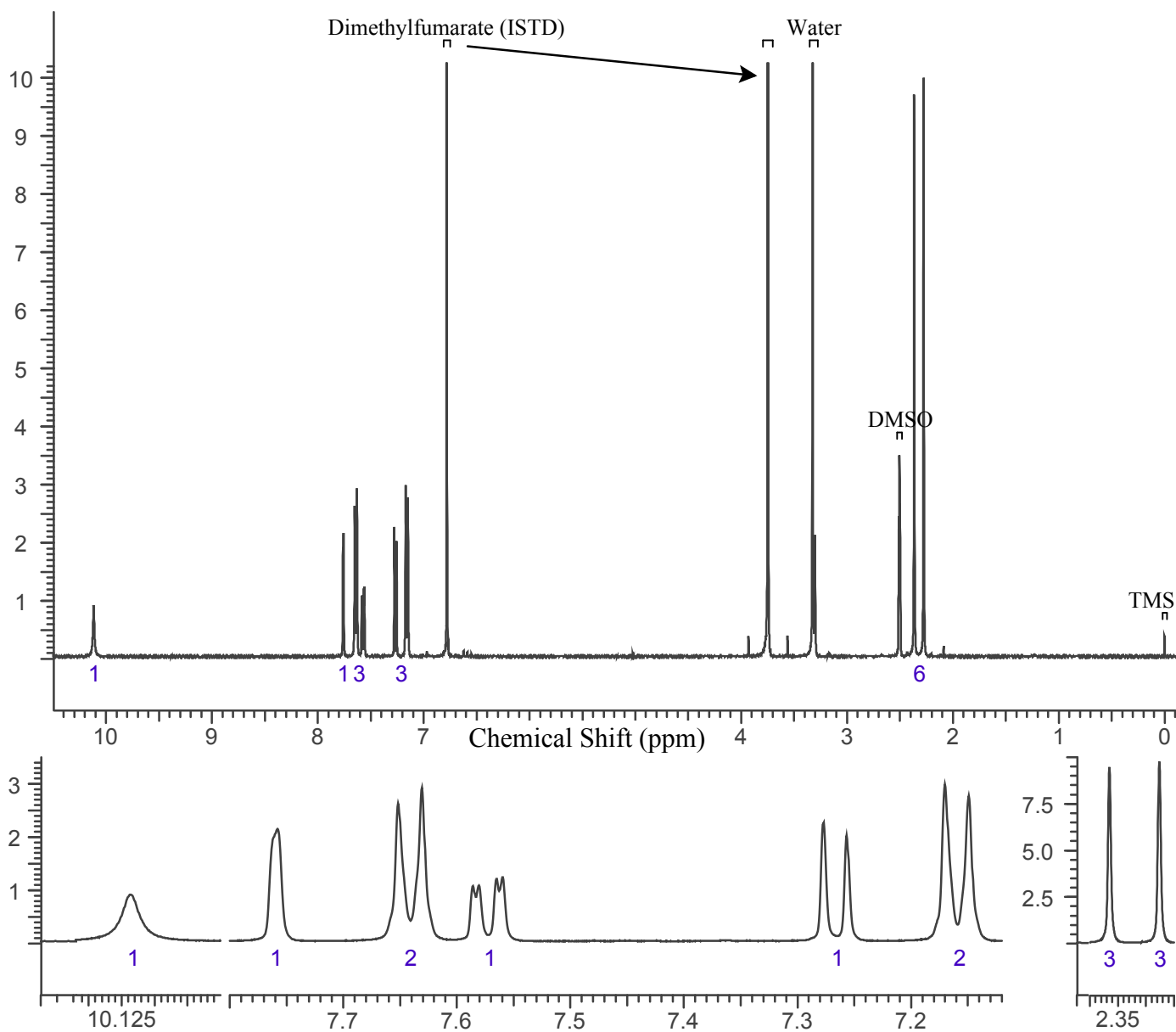
Instrument: 400 MHz NMR spectrometer

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

Pulse angle: 90°

Delay between pulses: 45 seconds

¹H NMR: URB-754; Lot 0438238-10; DMSO-*d*₆; 400 MHz



4.2 Gas Chromatography/Mass Spectrometry

Sample Preparation: Dilute analyte ~ 4 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 μ 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 16.0 min

Injection Parameters: Split Ratio = 25:1, 1 μ L injected

MS Parameters: Mass scan range: 34-550 amu

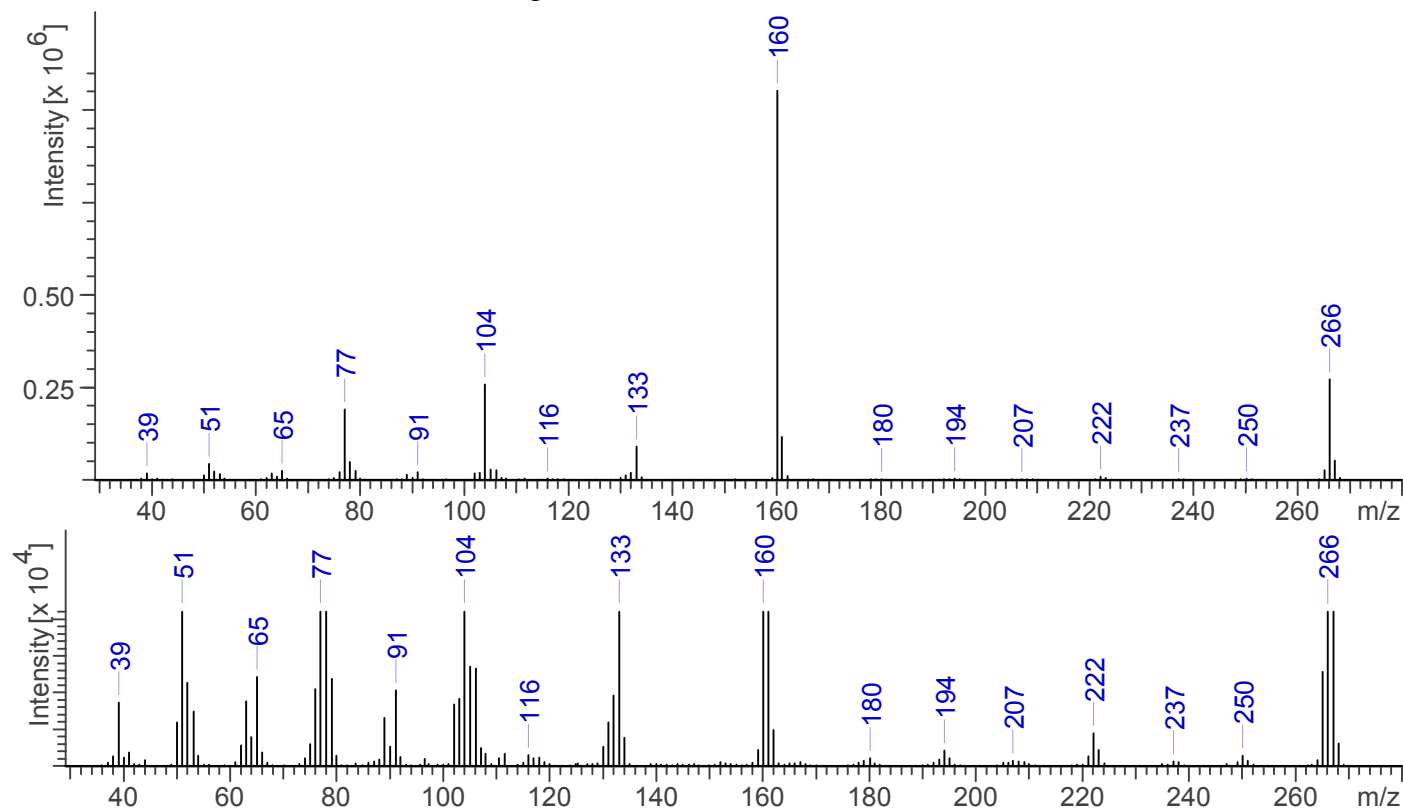
Threshold: 100

Tune file: stune.u

Acquisition mode: scan

Retention Time: 16.269 min

EI Mass Spectrum: URB-754; Lot 0438238-10



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⁻¹
Sample gain: 8
Aperture: 150

FTIR ATR (Diamond, 3 Bounce): URB-754; Lot 0438238-10

