1. GENERAL INFORMATION

**IUPAC Name:** 8-chloro-6-(2-fluorophenyl)-1-methyl-4H-benzo[f][1,2,4]triazolo[4,3-a][1,4]diazepine

**CAS#:** 28910-91-0

**Synonyms:** 8-chloro-6-(2-fluorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**UV\text{max}\text{(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>Base</td>
<td>C_{17}H_{12}ClFN_{4}</td>
<td>326.76</td>
<td>Not Determined</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~13 mg/mL in methanol-$d_4$ containing TMS for 0 ppm reference and maleic acid 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

$^1$HNMR: Flualprazolam; Lot# 0526790-11; CD3OD: 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in MeOH

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

**Column:** HP-5 MS (or equivalent); 30m x 0.25 mm x 0.25 μm

**Carrier Gas:** Helium at 1.5 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 280°C at 12 °C/min
3) Hold final temperature for 9.0 min

**Injection Parameters:**
- Split Ratio = 25:1
- 1 μL injected

**MS Parameters:**
- Mass scan range: 30-550 amu
- Threshold: 150
- Tune file: stune.u
- Acquisition mode: scan

**Retention Time:**
18.36 min

El Mass Spectrum: Flualprazolam; Lot# 0526790-11
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR with diamond ATR attachment (1 bounce)
Scan Parameters:
- Number of scans: 32
- Number of background scans: 32
- Resolution: 4 cm⁻¹
- Sample gain: 1
- Aperture: 150

FTIR ATR (Diamond 1 Bounce): Flualprazolam; Lot# 0526790-11