1. GENERAL INFORMATION

* **IUPAC Name:** 4-[2-(2,2,2-trifluoro-1-hydroxyethyl)pyrrolidin-1-yl]-2-(trifluoromethyl)benzonitrile
* **CAS#:** 1165910-22-4
* **Synonyms:** LGD-4033
* **Source:** DEA Reference Material Collection
* **Appearance:** White powder
* **$\text{UV}_{\text{max}}(\text{nm})$:** 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 ($^\circ$C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C$<em>{14}$H$</em>{12}$F$_6$N$_2$O</td>
<td>338.25</td>
<td>106.09</td>
</tr>
</tbody>
</table>
3. QUALITATIVE DATA

3.1 NUCLEAR MAGNETIC RESONANCE

Sample Preparation: Dilute analyte to ~14 mg/mL in methanol-$d_4$ 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

$^1$HNMR: LGD 4033; Lot# RM-170505-01; methanol-$d_4$; 400MHz
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

Sample Preparation: Dilute analyte ~4 mg/mL in 9:1 CHCl₃: 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: 250
  - Tune file: stune.u
  - Acquisition mode: scan
Retention Time: 12.29 min

EI Mass Spectrum: LGD 4033; Lot# RM-170505-01
3.3 INFRARED SPECTROSCOPY (FTIR)

Instrument: FTIR: Thermo-Scientific iS-10, Smart iTX

Scan Parameters:
- Number of scans: 32
- Number of background scans: 16
- Resolution: 4 cm\(^{-1}\)
- Sample gain: 1
- Aperture: 150

FTIR: Thermo-Scientific iS-10, Smart iTX: LGD 4033; Lot# RM-170505-01
4. ADDITIONAL RESOURCES