1. GENERAL INFORMATION

**IUPAC Name:** N-(naphthalen-1-yl)-1-pentyl-1H-indole-3-carboxamide

**CAS#:** 1338925-11-3

**Synonyms:** NNE1, NNEI, CBM-018

**Source:** DEA Reference Material Collection

**Appearance:** White powder

**$UV_{max} (\text{nm})$:** 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>$C_{24}H_{24}N_2O$</td>
<td>356</td>
<td>144.8</td>
</tr>
</tbody>
</table>
3. **QUALITATIVE DATA**

3.1 **NUCLEAR MAGNETIC RESONANCE**

*Sample Preparation:* Dilute analyte to ~20 mg/mL in DMSO 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

\(^1\text{H NMR: MN-24 Lot RM-140320-01, DMSO, 400MHz} \)
3.2 GAS CHROMATOGRAPHY/MASS SPECTROMETRY

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

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 µm
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) 90°C initial temperature for 2.0 min
    2) Ramp to 300°C at 14 °C/min
    3) Hold final temperature for 25.0 min

Injection Parameters: Split Ratio = 20:1, 1 µL injected
MS Parameters:
  - Mass scan range: 30-550 amu
  - Threshold: 100
  - Tune file: stune.u
  - Acquisition mode: scan

Retention Time: 26.141 min

3.3 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): MN-24 Lot RM-140320-01
4. ADDITIONAL RESOURCES

Forendex

Wikipedia