BATTELLE CERTIFICATE OF ANALYSIS

Name:	4-ANPP
Supplier:	Cerilliant
Catalog No.:	A-174
Lot #:	N/A
Chemical Formula:	$C_{19}H_{24}N_2$
Molecular Weight:	280.41

Analytical Results

Monoisotopic Exact Mass:	281.2012 (calc. for $[M+H]^+$) 281.2014 (obsd. ESI-MS)
Isotopic Purity:	N/A
Date of COA:	September 8, 2019

COA Prepared by: E. A. Lucas

505 King Avenue | Columbus, Ohio 43201-2696 | 614.424.7719 | lucasea@battelle.org | battelle.org

Figure 1: LC-QTOF Analysis of A-174

Table 1: LC-QTOF Conditions Used to Analyze A-174

Mass Spectrometer	Sciex TripleTOF 5600
UPLC Hardware	Waters Acquity I-Class
Mass Spectrometer Source	TurboIonSpray, Positive
Scan Ranges	TOF-MS: 50-1000 m/z MS/MS: 20-1000 m/z
UPLC Column	Waters Acquity BEH C18, 2.1 × 50 mm, 1.7 µm
Column Temperature	40°C
Mobile Phase A	0.1% Formic Acid in Water
Mobile Phase B	0.1% Formic Acid in Acetonitrile
Gradient Table	
Flow Rate	0.3 mL/min
Injection Volume	5 µL
Run Time	10 minutes

Time, min	%B
0 – 0.5	5
0.5 – 5	Ramp 5 to 100
5 – 5.5	100
5.51 – 10	5

Figure 2. GC-MS Chromatogram (EI, TIC) of A-174

Figure 3. Mass Spectrum (EI) of A-174 (Main Analyte)
Fragment Structure Assignments are Tentative and Unconfirmed

Table 2. GC-MS Conditions Used to Analyze A-174

Instrument	Agilent 6890 GC/5973 MSD
Carrier Gas:	Helium
Column:	Restek Rtx-5MS 30m x 0.25mm x 0.25um
Oven Program:	45°C hold for 1.0 min 20°C/min. to 320°C, hold for 15 min.
Total Run Time:	30 minutes
Transfer Line Temp.:	280°C
Injection:	Cool-on-column
Injection Port Temperature:	Tracking oven temperature
Carrier Flow Rate:	1.6 mL/min.
Injection Volume:	0.5 uL
Acquisition Mode:	EI
Scan Range:	35 to 500 amu
Electron Impact:	70 eV
MS Quad Temperature:	150°C
MS Source Temperature:	230°C

Figure 5. Low-resolution MS/MS (ESI, product ions of m/z 281) of A-174
Fragment Structure Assignments are Tentative and Unconfirmed

Table 3. LC-MS/MS-UV Conditions Used to Analyze A-174

<table>
<tr><td>Mass Spectrometer</td><td>Waters TQ-XS</td></tr>
<tr><td>UPLC Hardware</td><td>Waters Acquity I-Class</td></tr>
<tr><td>Mass Spectrometer Source</td><td>Electrospray, Positive Ionization</td></tr>
<tr><td>Photo Diode Array</td><td>Waters Acquity PDA</td></tr>
<tr><td>Scan Ranges</td><td>MS: 40-700 m/z
PDA: 210-300 nm</td></tr>
<tr><td>Mass Selected for MS/MS fragmentation</td><td>Observed mass ± 0.25 Da</td></tr>
<tr><td>UPLC Column</td><td>Phenomenex Prodigy ODS (3), 100mm x 2.0mm, 3µm</td></tr>
<tr><td>Column Temperature</td><td>50°C</td></tr>
<tr><td>Mobile Phase A</td><td>1% Formic Acid in Water</td></tr>
<tr><td>Mobile Phase B</td><td>1% Formic Acid in Acetonitrile</td></tr>
<tr><td>Gradient Table</td><td>
<table>
<tr><th>Time, min</th><th>%B</th><th>Flow, mL/min</th></tr>
<tr><td>0 – 1</td><td>2</td><td>0.3</td></tr>
<tr><td>1 – 11</td><td>Ramp 2 to 100</td><td>0.3</td></tr>
<tr><td>11.1 – 12</td><td>100</td><td>0.5</td></tr>
<tr><td>12.1 – 14</td><td>2</td><td>0.3</td></tr>
</table>
</td></tr>
<tr><td>Injection Volume</td><td>25 µL</td></tr>
<tr><td>Run Time</td><td>14 minutes</td></tr>
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