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ANALYTICAL REPORT

4-Anilinopiperidine (C11H16N2)

N-phenylpiperidin-4-amine

Remark – other active cpd. detected: none

Sample ID:	1758-17		
Sample description:	powder - white		
Sample type:	RM-reference material		
Comments ¹ :	; RESPONSE -purchasing		
Date of entry:	2/17/2017		

Substance identified- structure ² (base form)	
Systematic name:	N-phenylpiperidin-4-amine
Other names:	
Formula (per base form)	C11H16N2
M _w (g/mol)	176,26
Salt form:	HCI
StdInChIKey (for base form)	LKRMTUUCKBQGFO-UHFFFAOYSA-N
Other active cpd. detected	none
Add.info (purity)	98%

² Created by OPSIN free tool: <u>http://opsin.ch.cam.ac.uk/</u> **DOI:** 10.1021/ci100384d

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Report updates

date	comments (explanation)		

Supporting information

Analytical technique:	applied	remarks
GC-MS (El ionization)	+	NFL GC-RT (min): 4,93 BP(1): 83; BP(2): 82,BP(3) :93,
FTIR-ATR	+	direct measurement
GC-IR (condensed phase)	+	always as base form

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 ml and split mode (1:50). Injector temperature: 280 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 μ m. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 190 °C at rate 8 °C/min, then heating up to 293 0C at a rate of 18 °C/min, hold for 7.1 min, then heating at 50 °C/min up to 325 °C and finally 6.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadropole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. FTIR-ATR (Perkin Elmer): scan range 4000-400 cm⁻¹; resolution 4cm⁻¹

3. GC- (MS)-IR condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)

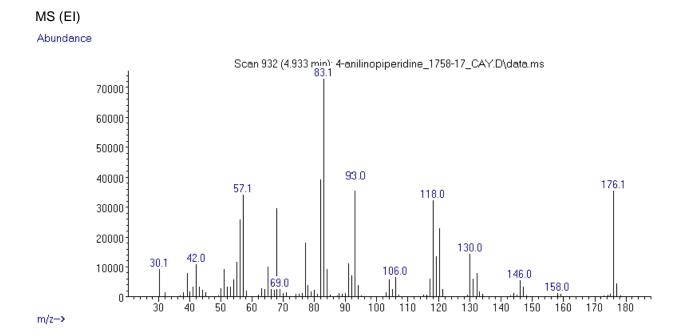
GC-method: Injection volume 1 ml and split mode (1:5). Injector temperature 280 $^{\circ}$ C. Chromatographic separation as above (1). Split MS : IR = 1 : 9.

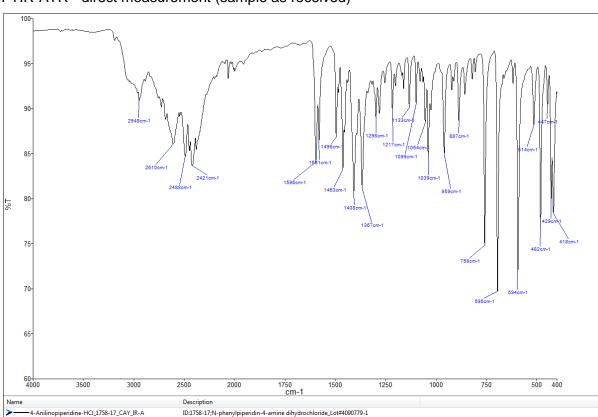
MSD source EI = 70 eV. GC-MS transfer line T= 235° C, source and quadropole temperatures 280° C and 180° C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.

IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm⁻¹.

4. HPLC-TOF for exact monoisotopic mass and empirical formula control - results are not shown in the report.

ANALYTICAL RESULTS







IR (condensed phase – after chromatographic separation)

