
Indoor air —

Part 39:

Determination of amines —

**Analysis of amines by (ultra-) high-
performance liquid chromatography
coupled to high resolution or tandem
mass spectrometry**

STANDARDSISO.COM : Click to view the full text of ISO 16000-39:2019



STANDARDSISO.COM : Click to view the full PDF of ISO 16000-39:2019



COPYRIGHT PROTECTED DOCUMENT

© ISO 2019

All rights reserved. Unless otherwise specified, or required in the context of its implementation, no part of this publication may be reproduced or utilized otherwise in any form or by any means, electronic or mechanical, including photocopying, or posting on the internet or an intranet, without prior written permission. Permission can be requested from either ISO at the address below or ISO's member body in the country of the requester.

ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Fax: +41 22 749 09 47
Email: copyright@iso.org
Website: www.iso.org

Published in Switzerland

Contents

	Page
Foreword	iv
Introduction	v
1 Scope	1
2 Normative references	1
3 Terms and definitions	2
4 Amines in indoor air	2
4.1 Properties of amines.....	2
4.2 Origin and occurrence of amines.....	2
5 Analytical procedure	2
5.1 Preparation of sample solutions.....	2
5.2 High-performance liquid chromatography.....	2
5.3 Tandem mass spectrometry.....	3
5.4 High resolution mass spectrometry.....	3
5.5 Sample sequence and external calibration.....	3
6 Testing of the suitability of the equipment and the instrumental analysis	3
6.1 General.....	3
6.2 High-performance or ultra-performance liquid chromatography (HPLC or UHPLC).....	3
6.3 Tandem mass spectrometry (MS-MS).....	4
6.4 High resolution mass spectrometry (HRMS).....	4
7 Reporting requirements	4
Annex A (informative) List of included amines	6
Annex B (informative) Performance data of the analytical method	9
Bibliography	12

Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights. Details of any patent rights identified during the development of the document will be in the Introduction and/or on the ISO list of patent declarations received (see www.iso.org/patents).

Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT) see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 146, *Air quality*, Subcommittee SC 6, *Indoor air*.

A list of all parts in the ISO 16000 series can be found on the ISO website.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

ISO 16000 (all parts) describe general requirements relating to the measurement of indoor air pollutants and the important conditions to be observed before or during the sampling of individual pollutants or groups of pollutants, as well as the measurements procedures themselves.

The definition of indoor environment is given by ISO 16000-1. Dwellings [living rooms, bedrooms, do-it-yourself (DIY) rooms, sport rooms and cellars, kitchens and bathrooms], workrooms or workplaces in buildings which are not subject to health and safety inspections with respect to air pollutants (e.g. offices, salesrooms), public buildings (e.g. restaurants, theatres, cinemas and other meeting rooms) and passenger cabins of motor vehicles and public transportation are among the most important types of indoor environment.

STANDARDSISO.COM : Click to view the full PDF of ISO 16000-39:2019

STANDARDSISO.COM : Click to view the full PDF of ISO 16000-39:2019

Indoor air —

Part 39:

Determination of amines — Analysis of amines by (ultra-) high-performance liquid chromatography coupled to high resolution or tandem mass spectrometry

1 Scope

This document, along with ISO 16000-38, specifies the measurement method for determining the mass concentration of primary, secondary and tertiary aliphatic and aromatic amines in indoor air using accumulated sampling and high-performance liquid chromatography (HPLC) coupled with tandem mass spectrometry (MS-MS) or high-resolution mass spectrometry (HRMS). The analytical procedure is covered by this document. The sampling procedure and the manufacturing of the samplers are covered by ISO 16000-38.

This document describes specifications for the chromatography and the mass spectroscopy for the amines. Measurement results are expressed in $\mu\text{g}/\text{m}^3$.

Although primarily intended for the measurement of amines listed in [Tables A.1](#) and [A.2](#), it can also be used for the measurement of other amines in indoor air. This document gives instructions and describes procedures for the inclusion of other amines.

The range of application of this document concerning the concentrations of amines in indoor air depends on the linear range of the calibration line and hence on the gas sample volume (here: from 5 l up to 100 l), the eluate volume (from 1 ml up to 5 ml), the injection volume (from 1 μl up to 10 μl) and the sensitivity of the analytical equipment (e.g. linear range from 2 pg up to 2 ng amine). The range of application can be expected to be from approximately 0,002 $\mu\text{g}/\text{m}^3$ (100 l sample) up to 2 000 $\mu\text{g}/\text{m}^3$ (5 l sample) for a common analytical equipment (e.g. Waters „TQD“) for the majority of the amines listed in [Tables A.1](#) and [A.2](#). The analysis of derivatives of ethanolamine is usually about 10 times more sensitive and the analysis of short-chained aliphatic amines is usually about 10 times less sensitive than the analysis of an average amine.

The performance data of the analytical method is given in Annex B, particularly in [Tables B.1](#) and [B.2](#).

This document can be used also for the determination of amines in water if the detection limit is sufficient.

This document does not cover the determination of isocyanates in indoor air (nor in water samples) as corresponding amines (covered by ISO 17734-1 and ISO 17734-2).

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 16000-38, *Indoor air — Part 38: Determination of amines in indoor and test chamber air — Active sampling on samplers containing phosphoric acid impregnated filters*

3 Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardisation at the following addresses:

- ISO online browsing platform: available at <http://www.iso.org/obp>
- IEC Electropedia: available at <http://www.electropedia.org/>

3.1 amines

nitrogen containing compounds with a sufficient vapor pressure ($>10^{-3}$ Pa) and a free electron pair at the nitrogen atom which can be protonated

4 Amines in indoor air

4.1 Properties of amines

Amines are basic and polar substances.

There are primary, secondary, tertiary, and quaternary amines.

Quaternary amines are not included in this document, as they have no free electron pair and therefore have very different properties. In this document the term “amines” refers only to primary, secondary, and tertiary amines.

Not protonated amines are oxidation sensitive.

Reaction of amines with acids results in ammonium salts of the amines. The ammonium salts are not oxidation sensitive.

4.2 Origin and occurrence of amines

Amines are produced by technical chemical processes and processing and in addition by biotic or abiotic decomposition of nitrogen compounds. Besides sources of biological origin, indoor air sources of amines could be, for instance, products containing polyurethane, especially foams, e.g. in vehicle seats, mattresses, pillows, and upholstered furniture or as thermal insulation or sound absorbing material. Several amines, in particular aromatic amines, are known as harmful compounds. Furthermore, most amines have an unacceptable odour in combination with a low odour threshold.

Further sources are for example food, e.g. fish (aliphatic amines), and cigarette smoke (aromatic amines).

5 Analytical procedure

5.1 Preparation of sample solutions

ISO 16000-38 describes the procedure to get the aqueous eluate of the ammonium salts of the sampled amines. The sample solution (which contains already approximately $0,02 \mu\text{mol}/\mu\text{l}$ up to $0,1 \mu\text{mol}/\mu\text{l}$ phosphoric acid) can be used for the injection into the HPLC system without further treatment.

5.2 High-performance liquid chromatography

- stationary phase of separating column: pentafluorophenyl;
- common column dimensions: length 150 mm, inner diameter: 2,1 mm;

- common particle size: 3 µm (HPLC), 1,7 µm [Ultra Performance Liquid Chromatography (UHPLC)];
- column temperature: 40 °C;
- injection volume: 1 µl to 10 µl;
- mobile phase: acetonitrile and water with each 0,02 % formic acid (500 µl formic acid in 2,5 l acetonitrile or 2,5 l water, respectively);
- mobile phase composition: 28 % acetonitrile/72 % water, isocratic.

5.3 Tandem mass spectrometry

- ionisation: electrospray ionisation, positive mode (ESI+);
- source temperature: 120 °C;
- desolvation gas: nitrogen, 900 l/h;
- desolvation temperature: 420 °C;
- cone gas: nitrogen, 50 l/h;
- precursor ion: M+1;
- collision gas: argon;
- calibration: external and additionally with Pyridine-d5 as internal standard.

5.4 High resolution mass spectrometry

- ionisation: electrospray ionisation, positive mode (ESI+).

5.5 Sample sequence and external calibration

- external calibration: run calibration standards at least at the beginning and at the end of a sample sequence;
- every 25 samples or less and at the beginning and end, run a calibration blank and a calibration check solution of an independent source;
- every 50 samples (for example) and at the end of a run, analyse an interference check solution (ICS).

6 Testing of the suitability of the equipment and the instrumental analysis

6.1 General

In [Table A.3](#), several amines are listed which can interfere with another amine in the instrumental analysis. In order to check and confirm the suitability of the selected system and procedure following issues have to be tested.

6.2 High-performance or ultra-performance liquid chromatography (HPLC or UHPLC)

The chromatographic separation of following compounds has to be tested and confirmed:

- a) Diethylamine (11) and N,N-Dimethylethylamine (24);
- b) Isobutylamine (2) and n-Butylamine (10);
- c) 2-(Dimethylamino)ethanol (8) and 2-(Ethylamino)ethanol (25);

d) Diisobutylamine (14) and Di-n-butylamin (16).

Usually 4-Ethylmorpholine (4) and 2-(Diethylamino)ethanol (3) as well as Morpholine (13) and 2-(Dimethylamino)ethanol (8) cannot be separated sufficiently on pentafluorophenyl terminated stationary phases. These compounds have to be distinguished by high resolution or tandem mass spectrometry.

The chromatographic separation of Diethylamine (11) and N,N-Dimethylethylamine (24) is not always possible (depends mainly on the column). If tandem mass spectrometry is used for detection the ratio of the product ions (46 and 29 u/e; 6.3) can be used for discrimination.

6.3 Tandem mass spectrometry (MS-MS)

The selectivity of the tandem mass spectrometry has to be tested and confirmed for following potentially interfering amines or product ions, respectively:

	Relevant product ions
a) Diethylamine (11) and N,N-Dimethylethylamine (24):	ratio of 46 and 29 u/e
b) 2-(Dimethylamino)ethanol (8) and Morpholine (13):	ratio of 72, 70, 45 and 44 u/e
c) 2-(Ethylamino)ethanol (25) and Morpholine (13):	ratio of 72, 70, 45 and 44 u/e
d) 4-Ethylmorpholine (4) and 2-(Diethylamino)ethanol (3):	ratio of 100, 72, 45 and 44 u/e

For additional information see [Annex A \(Tables A.3 and A.4\)](#).

6.4 High resolution mass spectrometry (HRMS)

A possible interference due to a loss of H₂ during ionization has to be tested and excluded for following compounds:

- Morpholine (13) by 2-(Dimethylamino)ethanol (8);
- Morpholine (13) by 2-(Ethylamino)ethanol (25);
- 4-Ethylmorpholine (4) by 2-(Diethylamino)ethanol (3).

7 Reporting requirements

- reference to this document (ISO 16000-39);
- reason of the measurement (e.g. peculiar odour, product quality testing, process control);
- identification of the sample (distinct sample number);
- sample description (origin, e.g. active sampling of air referred to ISO 16000-38 in an office, a test chamber, car or manufacturing plant and subsequent elution with water);
- if appropriate, reference to ISO 16000-38, otherwise detailed description of the sampler and the sampling procedure;
- date and time of sampling;
- short description of the location of sampling;
- sampling conditions: relative humidity, temperature and pressure;
- volume of sampled air (in l);

- if appropriate: description of transportation and storage of the loaded sampler;
- applied eluent volume (elution of the amines and the phosphoric acid from the sampler referred to ISO 16000-38);
- if appropriate: description of (further) sample preparation (e.g. subsequent dilution);
- short description of the instrumental analysis (e.g. MS/MS or HRMS);
- target analytes with CAS number;
- limit of detection and limit of quantification in the analysed solution in $\mu\text{g/l}$ and in the air sample in $\mu\text{g/m}^3$ for all target analytes;
- mass concentration of all target analytes in the analysed solution in $\mu\text{g/l}$ with 3 significant digits, where necessary specify “below limit of quantification”;
- mass concentration of all target analytes in the air sample in $\mu\text{g/m}^3$ with 2 significant digits;
- measurement uncertainty;
- if appropriate, further necessary specifications and details.

Annex A (informative)

List of included amines

Table A.1 — List of amines with toxicological relevance

Consecutive number	CAS number	Amine	GHS 06	GHS 08
1	62-53-3	Aniline	X	X
2	78-81-9	Isobutylamine	X	—
3	100-37-8	2-(Diethylamino)ethanol	X	—
4	100-74-3	4-Ethylmorpholine	X	—
5	100-97-0	Hexamethylenetetramine ^a	—	—
6	103-83-3	N,N-Dimethylbenzylamine	X	—
7	106-49-0	p-Toluidine	X	X
8	108-01-0	2-(Dimethylamino)ethanol	X	—
9	108-91-8	Cyclohexylamine	X	X
10	109-73-9	n-Butylamine	X	—
11	109-89-7	Diethylamine	X	—
12	110-89-4	Piperidine	X	—
13	110-91-8	Morpholine	X	—
14	110-96-3	Diisobutylamine	X	—
15	111-42-2	Diethanolamine	—	X
16	111-92-2	Di-n-butylamine	X	—
17	121-44-8	Triethylamine	X	—
18	616-47-7	1-Methylimidazole	X	—
19	872-50-4	1-Methyl-2-pyrrolidinone	—	X
20	2687-91-4	1-Ethyl-2-pyrrolidinone	—	X
21	3033-62-3	[Bis(2-dimethylamino)ethyl]ether	X	—
22	280-57-9	1,4-Diazabicyclo[2.2.2]octane ^b		

^a Hexamethylenetetramine is a source of formaldehyde.

^b Used to test the samplers.

Table A.2 — List of further amines

Consecutive number	CAS number	Amine	GHS 06	GHS 08	purpose (reason)
23	7291-22-7	Pyridine-d5	—	—	internal standard
24	598-56-1	N,N-Dimethylethylamine	—	—	interference with 11
25	110-73-6	2-(Ethylamino)ethanol	—	—	interference with 8 and 13

Table A.3 — List of interfering amines

Consecutive number	CAS number	Amine	GHS 06	GHS 08	interference group	mass transition
24	598-56-1	N,N-Dimethylethylamine	—	—	a1	74 > 46 (29)
11	109-89-7	Diethylamine	X	—	a1	74 > 29 (46)
2	78-81-9	Isobutylamine	X	—	a2	74 > 57
10	109-73-9	n-Butylamine	X	—	a2	74 > 57
8	108-01-0	2-(Dimethylamino)ethanol	X	—	b	90 > 72 (45)
25	110-73-6	2-(Ethylamino)ethanol	—	—	b	90 > 72 (45)
13	110-91-8	Morpholine	X	—	b	88 > 70 ^a (44) ^a
3	100-37-8	2-(Diethylamino)ethanol	X	—	c	118 > 100 ^a (45)
4	100-74-3	4-Ethylmorpholine	X	—	c	116 > 72 (44)
14	110-96-3	Diisobutylamine	X	—	d	130 > 57 (74)
16	111-92-2	Di-n-butylamine	X	—	d	130 > 74 (57)

^a This compound/mass transition usually can be measured without interference.

Interference group a

The amines of group a1 usually can be easily separated from amines of group a2 by chromatography.

Interference group a1

The chromatographic separation of N,N-Dimethylethylamine (24) and Diethylamine (11) is challenging. If tandem MS is used the proportion of the peak area of the mass transitions 74 > 29 and 74 > 46 can be used additionally to distinguish between amine 24 and 11.

Interference group a2

The chromatographic separation of Isobutylamine (2) and n-Butylamine (10) is challenging. Tandem MS cannot be used to distinguish between amine 2 and 10, therefore a sufficient chromatographic peak separation is essential.

Interference group b

In interference group b Morpholine (13) can be distinguished from 2-(Dimethylamino)ethanol (8) and 2-(Ethylamino)ethanol (25) by mass spectrometry. MS cannot be used to distinguish between 8 and 25, therefore a sufficient peak separation in chromatography is essential.

Interference group c

Experimental data show that 2-(Diethylamino)ethanol (3) and 4-Ethylmorpholine (4) usually cannot be separated by a pentafluorophenyl terminated column, therefore they have to be distinguished by mass spectrometry.

2-(Diethylamino)ethanol (3) can be detected without interference from 4-Ethylmorpholine (4).

The concentration of 4-Ethylmorpholine (4) has to be corrected subsequently.

Interference group d

Diisobutylamine (14) and Di-n-butylamine (16) usually can be separated by chromatography easily.

Table A.4 — List of amines with mass transition data

Consecutive number	CAS number	Amine	M1 = M+H ⁺	M2	M3	Interference group ^a
24	598-56-1	N,N-Dimethylethylamine	74	46	29	a1
11	109-89-7	Diethylamine	74	29	46	a1
2	78-81-9	Isobutylamine	74	57	—	a2
10	109-73-9	n-Butylamine	74	57	—	a2
18	616-47-7	1-Methylimidazole	83	56	28	—
22	7291-22-7	Pyridine-d5	85	58	—	—
12	110-89-4	Piperidine	86	30	69	—
13	110-91-8	Morpholine	88	70	44	b
8	108-01-0	2-(Dimethylamino)ethanol	90	72	45	b
25	110-73-6	2-(Ethylamino)ethanol	90	72	45	b
1	62-53-3	Aniline	94	77	—	—
19	872-50-4	1-Methyl-2-pyrrolidinone	100	69	58	—
9	108-91-8	Cyclohexylamine	100	83	55	—
17	121-44-8	Triethylamine	102	74	—	—
15	111-42-2	Diethanolamine	106	88	45	—
7	106-49-0	p-Toluidine	108	91	93	—
23	280-57-9	1,4-Diazabicyclo[2.2.2]octane	113	84	56	—
20	2687-91-4	1-Ethyl-2-pyrrolidinone	116	85	69	—
4	100-74-3	4-Ethylmorpholine	116	72	44	c
3	100-37-8	2-(Diethylamino)ethanol	118	100	45	c
14	110-96-3	Diisobutylamine	130	57	74	d
16	111-92-2	Di-n-butylamine	130	74	57	d
6	103-83-3	N,N-Dimethylbenzylamine	136	91	—	—
5	100-97-0	Hexamethylenetetramine [#]	141	112	42	—
21	3033-62-3	[Bis(2-dimethylamino)ethyl]ether	161	72	116	—

^a Interference group (Table A.3).

Annex B (informative)

Performance data of the analytical method

The sensitivity of the analytical method depends on the gas sample volume $V_{\text{gas sample}}$ (from 5 l up to 100 l), the eluate volume V_{eluate} (from 1 ml up to 5 ml), the injection volume $V_{\text{injection}}$ (from 1 μl up to 10 μl) and the sensitivity of the analytical equipment.

The injected mass m_{injected} [pg] of an amine can be calculated from the concentration c_{air} [$\mu\text{g}/\text{m}^3$] in the air sample by [Formula \(B.1\)](#):

$$m_{\text{injected}} [\text{pg}] = c_{\text{air}} \left[\frac{\mu\text{g}}{\text{m}^3} \right] \cdot \frac{V_{\text{gas sample}} [\text{l}]}{V_{\text{eluate}} [\text{ml}]} \cdot V_{\text{injection}} [\mu\text{l}] \quad (\text{B.1})$$

According to [Formula \(B.1\)](#) a concentration of 1 $\mu\text{g}/\text{m}^3$ corresponds to 1 000 pg injected mass for the highest gas sample volume of 100 l, the lowest eluate volume of 1 ml and the highest injection volume of 10 μl :

$$m_{\text{injected}} [\text{pg}] = 1 \frac{\mu\text{g}}{\text{m}^3} \cdot \frac{100 \text{ l}}{1 \text{ ml}} \cdot 10 \mu\text{l} = 1\,000 \text{ pg}$$

Therefore the sensitivity of the analytical equipment should be at least 1 000 pg for the limit of quantification (LOQ).

[Table B.1](#) exemplifies the limit of detection (LOD), the limit of identification (LOI) and the limit of quantification (LOQ) in [pg] plus the ideal and acceptable regression method for the amines of [Table A.1](#). In the example ([Table B.1](#)) the sensitivity of the analytical equipment varies from 80,3 pg (LOQ) for n-Butylamine down to 4,3 pg (LOQ) for 4-Ethylmorpholine.

The concentration c_{air} [$\mu\text{g}/\text{m}^3$] in the air sample can be calculated from the detected mass m_{detected} [pg] by [Formula \(B.2\)](#):

$$c_{\text{air}} \left[\frac{\mu\text{g}}{\text{m}^3} \right] = \frac{m_{\text{detected}} [\text{pg}]}{V_{\text{injection}} [\mu\text{l}]} \cdot \frac{V_{\text{eluate}} [\text{ml}]}{V_{\text{gas sample}} [\text{l}]} \quad (\text{B.2})$$

According to [Formula \(B.2\)](#) a detected mass of 80 pg corresponds to a concentration of 0,32 $\mu\text{g}/\text{m}^3$ in the air sample for a gas sample volume of 50 l, an eluate volume of 1 ml and an injection volume of 5 μl :

$$c_{\text{air}} \left[\frac{\mu\text{g}}{\text{m}^3} \right] = \frac{80 \text{ pg}}{5 \mu\text{l}} \cdot \frac{1 \text{ ml}}{50 \text{ l}} = 0,32 \frac{\mu\text{g}}{\text{m}^3}$$

[Table B.2](#) exemplifies the limit of detection (LOD), the limit of identification (LOI) and the limit of quantification (LOQ) in [$\mu\text{g}/\text{m}^3$] in the air sample for the amines of [Table A.1](#) for a gas sample volume of 50 l, an eluate volume of 1 ml and an injection volume of 5 μl . In the example ([Table B.2](#)) the sensitivity of the analytical method varies from 0,32 $\mu\text{g}/\text{m}^3$ (LOQ) for n-Butylamine down to 0,02 $\mu\text{g}/\text{m}^3$ (LOQ) for 4-Ethylmorpholine.

Table B.1 — Limit of detection (LOD), limit of identification (LOI) and limit of quantification (LOQ) of an exemplary analytical system in [pg] plus ideal and acceptable regression method for the amines of Table A.1.

Con. num.	Amines	MS/MS-system*	Injected mass [pg]			Ideal regression: linear/quadr.	Linear regression acceptable?
			LOD	LOI	LOQ		
1	Aniline	TQD	3,1	6,1	9,3	linear	yes
2	Isobutylamine	TQ-S	7,5	15,0	24,4	linear	yes
3	2-(Diethylamino)ethanol	TQD	3,1	6,2	9,4	linear	yes
4	4-Ethylmorpholine	TQD	1,3	2,7	4,3	linear	yes
5	Hexamethylenetetramine	—	—	—	—	—	—
6	N,N-Dimethylbenzylamine	TQD	2,1	4,2	6,6	linear	yes
7	p-Toluidine	—	—	—	—	—	—
8	2-(Dimethylamino)ethanol	TQD	3,9	7,8	11,9	linear	yes
9	Cyclohexylamine	TQD	3,2	6,4	9,7	linear	yes
10	n-Butylamine	TQD	22,8	45,6	80,3	quadratic	yes
11	Diethylamine	TQD	29,1	58,2	41,5	quadratic	yes
		TQ-S	7,8	15,5	25,1	linear	yes
12	Piperidine	TQD	7,8	15,6	20,3	linear	yes
13	Morpholine	TQD	9,8	19,5	21,0	quadratic	yes
14	Diisobutylamine	TQD	6,8	13,6	22,4	linear	yes
15	Diethanolamine	—	—	—	—	—	—
16	Di-n-butylamine	TQD	2,8	5,7	8,8	linear	yes
17	Triethylamine	TQD	11,4	22,7	28,1	quadratic	yes
18	1-Methylimidazole	TQD	5,0	10,0	13,9	linear	yes
19	1-Methyl-2-pyrrolidinone	TQD	26,7	53,5	29,7	quadratic	yes
		TQ-S	3,0	6,1	10,9	linear	yes
20	N-Ethyl-2-pyrrolidinone	TQD	2,6	5,2	7,9	linear	yes
21	[Bis-(2-dimethyl-amino)ethyl]ether	TQD	5,4	10,8	14,8	linear	yes
22	1,4-Diazabicyclo[2.2.2]octane	TQD	5,1	10,1	14,6	quadratic	yes
		TQ-S	3,9	7,7	13,4	linear	yes

* TQD: Waters® Xevo® TQD, TQ-S: Waters® Xevo® TQ-S

Table B.2 — Limit of detection (LOD), limit of identification (LOI), limit of quantification (LOQ) in the air sample in [µg/m³] for the amines of Table A.1.

Consecutive number	Amines	MS/MS-system*	Concentration in the air sample# [µg/m³]		
			LOD	LOI	LOQ
1	Aniline	TQ-D	0,01	0,02	0,04
2	Isobutylamine	TQ-S	0,03	0,06	0,10
3	2-(Diethylamino)ethanol	TQD	0,01	0,02	0,04
4	4-Ethylmorpholine	TQD	0,01	0,01	0,02
5	Hexamethylenetetramine	—	—	—	—

* TQD: Waters® Xevo® TQD, TQ-S: Waters® Xevo® TQ-S

Air sample volume: 50 l, eluent volume: 1 ml, injection volume: 5 µl