



iMethod™ Test for Ethanolamines Version 1.0 for Cliquid® Software

iMethod™ Tests are pre-configured and verified LC/MS/MS methods that reduce the need for method development and save you weeks of time and effort—and thousands of dollars—in the deployment of a new assay.

Ethanolamines have been used as bio- and environmental markers for nitrogen mustards to measure potential exposures. Direct quantification of exposure to nitrogen mustards (HN1, HN2 and HN3) is difficult due to their instability¹. Ethanolamines are also manufactured in large volume (over a million tons per year) and have a wide range of both industrial and domestic uses such as pesticide manufacturing, emulsifying agents and detergents, and in bactericides and cosmetics². To monitor the removal of ethanolamines from industrial discharged waste water and the extent of human and environmental exposure to nitrogen mustards, a quantitative analytical method is desired.

Reported analytical methods for ethanolamines quantitation include chromatographic separation with mass spectrometric

detection. Gas chromatography methods with derivatization limit the method throughput and liquid chromatography methods with reverse phase columns suffer from poor retention and resolution.

This iMethod Test is an ultra high performance liquid chromatography tandem mass spectrometric (uHPLC-MS/MS) method using the Dionex UltiMate 3000 Rapid Separation LC system (RSLC) with an AB SCIEX 4000 QTRAP® or API 4000™ LC/MS/MS System. A Dionex Acclaim Trinity P1 mixed mode column featuring reverse phase and cation exchange retention mechanisms is used to provide retention and resolution for all analytes within five minutes. The MS/MS system is operated in MRM mode to ensure sensitive and selective detection.

Figure 1. MRM Chromatogram of ethanolamines at 0.5 ppb

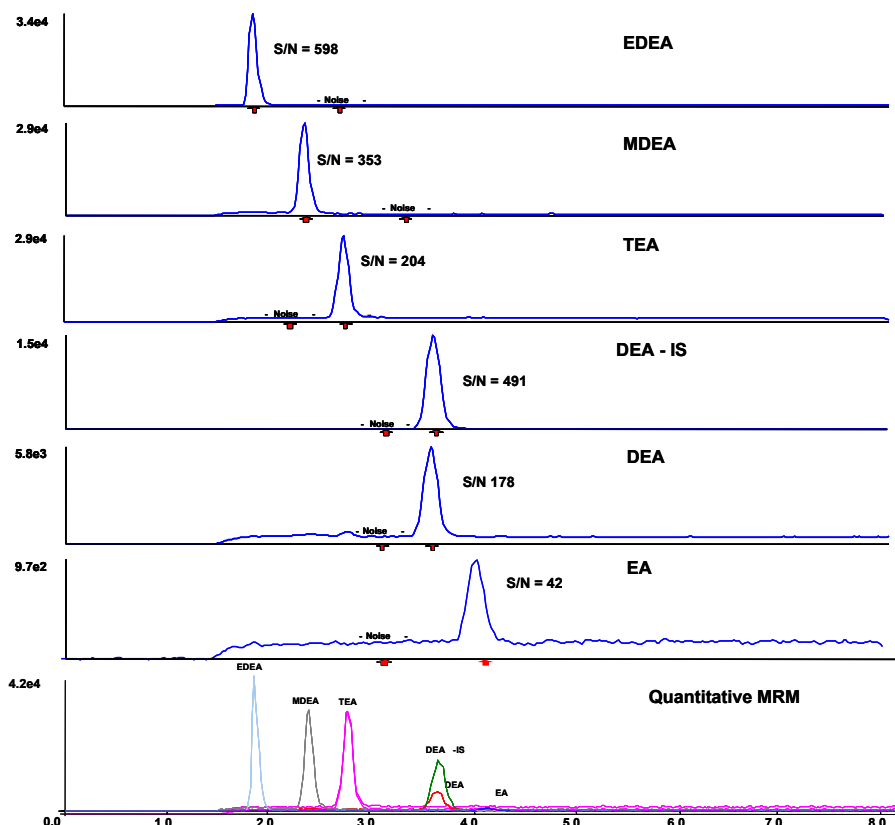


Table 1. Calibrations, accuracy, %RSD, and method detection limits for ethanolamines

Analyte	ID	r	%Accuracy* at 0.5 ppb	%RSD**	MDL*** (ppb)	LOQ (ppb)	S/N at LOQ
<i>N-Ethyldiethanolamine</i>	EDEA	0.9993	92.6	3.58	0.052	0.05	107
<i>N-Methyldiethanolamine</i>	MDEA	0.9996	96.8	3.26	0.050	0.05	54.5
<i>Triethanolamine</i>	TEA	0.9994	106	5.49	0.092	0.05	26.0
<i>Diethanolamine</i>	DEA	0.9999	102	3.85	0.061	0.05	24.9
<i>Ethanolamine</i>	EA	0.9990	102	5.34	0.085	0.20	13.1

* Accuracy was calculated by (observed amount/specified amount) ×100%.

** %RSD was calculated from 7 replicate injection at 0.5 ppb.

*** MDL was calculated by $MDL = s \times t$, where s is the standard deviation of the seven replicate injection at 0.5 ppb, and t is the student's t at 99% confidence interval.

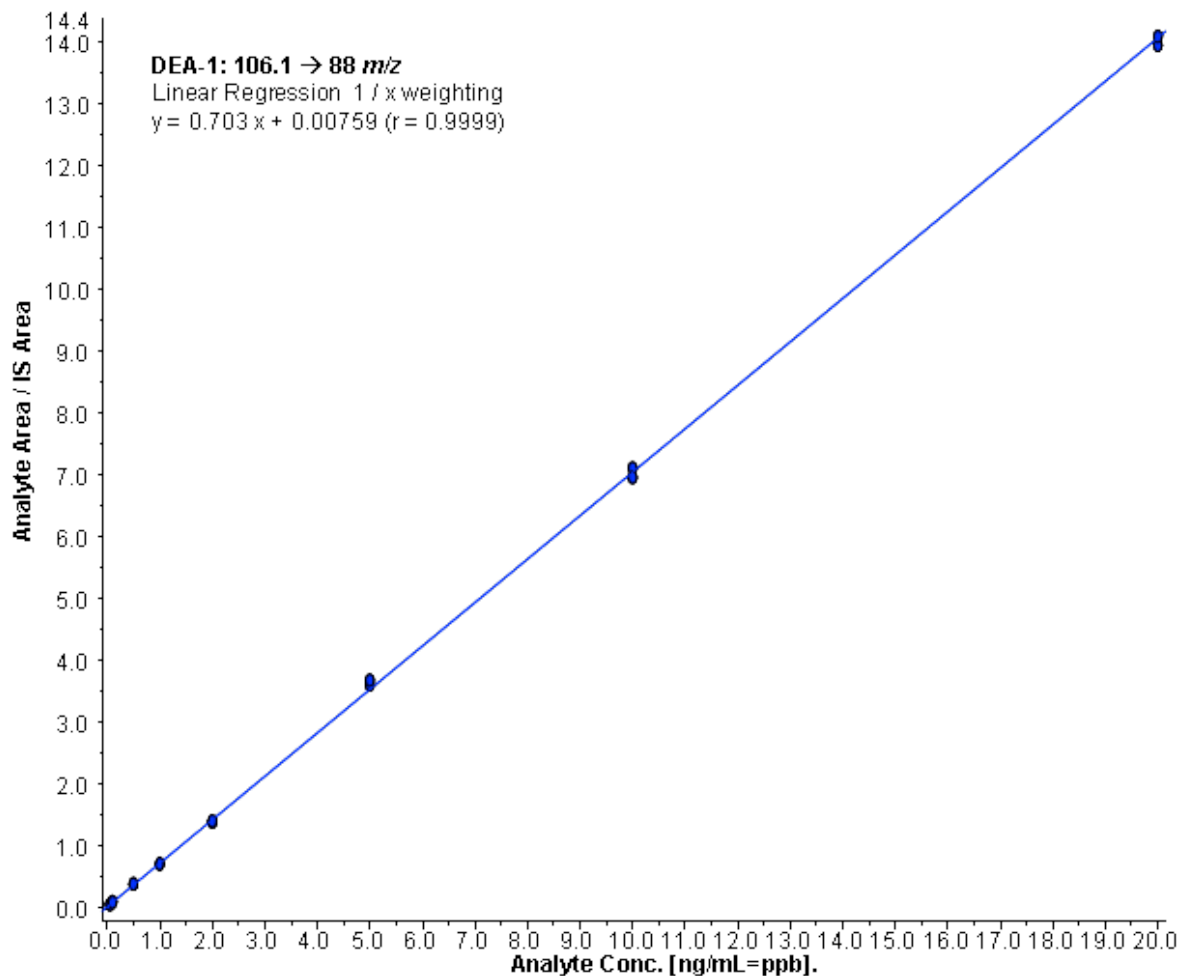


Figure 2. Calibration curve of DEA (0.05 – 20 ppb), in deionized water

System Requirements

- AB SCIEX 4000 QTRAP® or API 4000™ LC/MS/MS System
- Dionex UltiMate 3000 RSLC system
 - DGP-3600RS dual gradient pump
 - SRD-3600 solvent rack with 6-channel online degasser
 - TCC-3000RS column oven with 6-port two-position switching valve
 - WPS-3000TRS thermostated split loop autosampler
- Separation Column
 - Dionex Acclaim Trinity P1 column (2.1 × 100 mm, 3 µm, P/N 071389)
- Ethanolamines standards, Sigma-Aldrich (www.sigmaaldrich.com)
- Internal standard, DEA – d8, C/D/N Isotopes (www.cdnisotopes.com) D5308

Ordering Information

Product Name	Part Number
iMethod™ Test for Ethanolamines in Water Version 1.1 for Cliquid® Software	5011870

While the information provided above outlines the instrument requirements and expected results obtainable from the AB SCIEX iMethod™ Test for the Analysis of Ethanolamines in water, please note that the results obtained do require some experience with LC/MS/MS and sample preparation procedures. As such, web-based and on-site training are available to assist in the deployment of the iMethod™ Test and are recommended for inexperienced users. Please consult your local sales representative for more details.

Important Note

The iMethod™ Test described above has been designed by AB SCIEX to provide the sample prep and instrument parameters required to accelerate the adoption of this method for routine testing. This method is provided for information purposes only. The performance of this method is not guaranteed due to many different potential variations, including instrument performance, tuning, and maintenance, chemical variability and procedures used, technical experience, sample matrices, and environmental conditions. It is up to the end user to make adjustments to this method to account for slight differences in equipment and/or materials from lab to lab as well as to determine and validate the performance of this method for a given instrument and sample type. Please note that a working knowledge of Analyst® Software may be required to do so.

The purchase and use of certain of the chemicals listed below may require the end user to possess any necessary licenses, permits or approvals, if such are required in accordance with local laws and regulations. It is the responsibility of the end user to purchase these chemicals from a licensed supplier, if required in accordance with local laws and regulations. The suppliers and part numbers listed below are for illustrative purposes only and may or may not meet the aforementioned local requirements. AB SCIEX is not responsible for user's compliance with any statute or regulation, or for any permit or approval required for user to implement any iMethod procedure.

The information included in this product is intended for reference and research purposes only. AB SCIEX offers no guarantee as to the quality or suitability of this data and suitability of the information included in this (Library, database, etc.) for use with your specific application.

1. Black, R.M.; Read, R.W., J. Chromatogr., A 1998, 449, 261–270.
2. Edser, C., Focus on Surfactants 2004, 7, 1–2.

For Research Use Only. Not for use in diagnostic procedures.

© 2011 AB SCIEX. The trademarks mentioned herein are the property of AB Sciex Pte. Ltd. or their respective owners. AB SCIEX™ is being used under license.

Publication number: 24200211-01