

M. Palmer, E. Claude, M. Snel
Waters Corporation, MS technologies Center, UK

INTRODUCTION

Mass resolution is the ability to separate two adjacent masses. It defines the performance of an analyzer and is a measure of the extent to which adjacent ions can be distinguished from each other with less than a defined amount of overlap. For a single peak this can be calculated from the width of a peak at a defined height and is usually referred to as Full Width Half Maximum (FWHM). FWHM is the resolution measured with a 50% valley overlap between peaks of adjacent m/z.

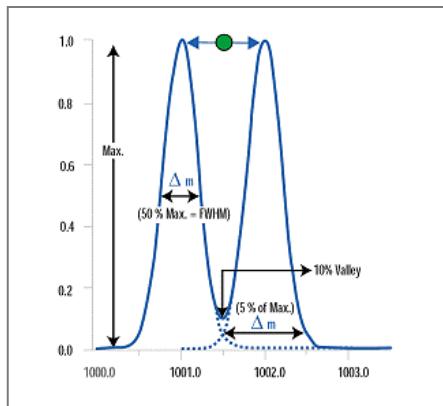


Figure 1. Definition of FWHM for a mass spectral peak

Resolution can be calculated using the following equation:

$$\text{Resolution} = \frac{m}{\Delta m}$$

where m is the observed m/z and Δm is the measured width at half peak height. Two key advantages of increasing resolution are:

- Increased ability to separate peaks which are close in m/z
- Improved detection limits through the generation of narrower, taller peaks.

It is often assumed that high resolution is always required for good mass accuracy, this has however been shown not to be the case¹.

EXPERIMENTAL

The resolving power of the Waters® Micromass® MALDI micro MX™ is demonstrated in reflectron and linear mode, in positive ion and negative ion modes.

Resolution reflectron mode

Sample: Adrenocorticotrophic hormone clip 18 – 39 (ACTH) at a concentration of 2 pmol/µL in 0.1% trifluoroacetic acid (TFA).

Matrix: Purified α-cyano-4-hydroxy cinnamic acid matrix was obtained from Waters (186002331). Matrix was prepared at 2 mg/mL in 1:1 acetonitrile:aqueous 0.1% TFA.

Samples were mixed 1:1 with matrix and 1 µL was spotted directly onto the target plate and allowed to air dry prior to analysis.

Data acquisition: Six separate acquisitions in positive and negative mode.

Resolution linear mode

Sample: Cytochrome C (equine) at a concentration of 2 pmol/µL in 0.1% TFA.

Matrix: The matrix was prepared and used in 2 stages, •10 mg/mL sinapinic acid in acetone (*Matrix 1*) •10 mg/mL sinapinic acid in 60:40 aqueous 0.1% TFA:acetonitrile (*Matrix 2*).

1 µL of *Matrix 1* was applied to the target plate and allowed to air dry then *Matrix 2* was mixed 1:1 with the sample and 1 µL was spotted on top of the *Matrix 1* thin film.

Data acquisition: Six separate acquisitions in positive and negative mode.

RESULTS

The results obtained are summarised in Table 1. Examples for each mode are shown in Figures 2-5. The MALDI micro MX exceeded the specified resolution in every mode.

Mode	Polarity	Average resolution (six acquisitions)	Instrument specification
Reflectron	positive	14,158	10,000
Reflectron	negative	11,354	10,000
Linear	positive	1,082	1,000
Linear	negative	1,124	1,000

Table 1. Average resolution over six acquisitions.

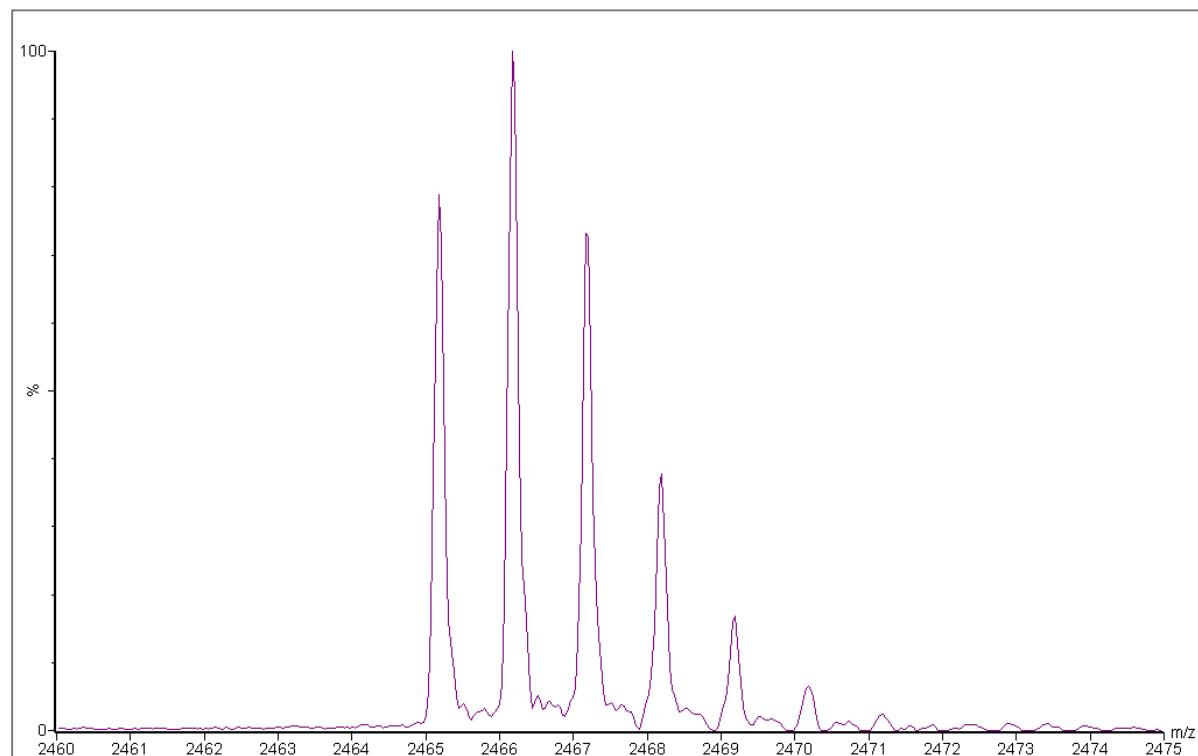


Figure 2. Example of resolution in reflectron mode (positive). Observed resolution $\approx 16,000$.

Technical NOTE

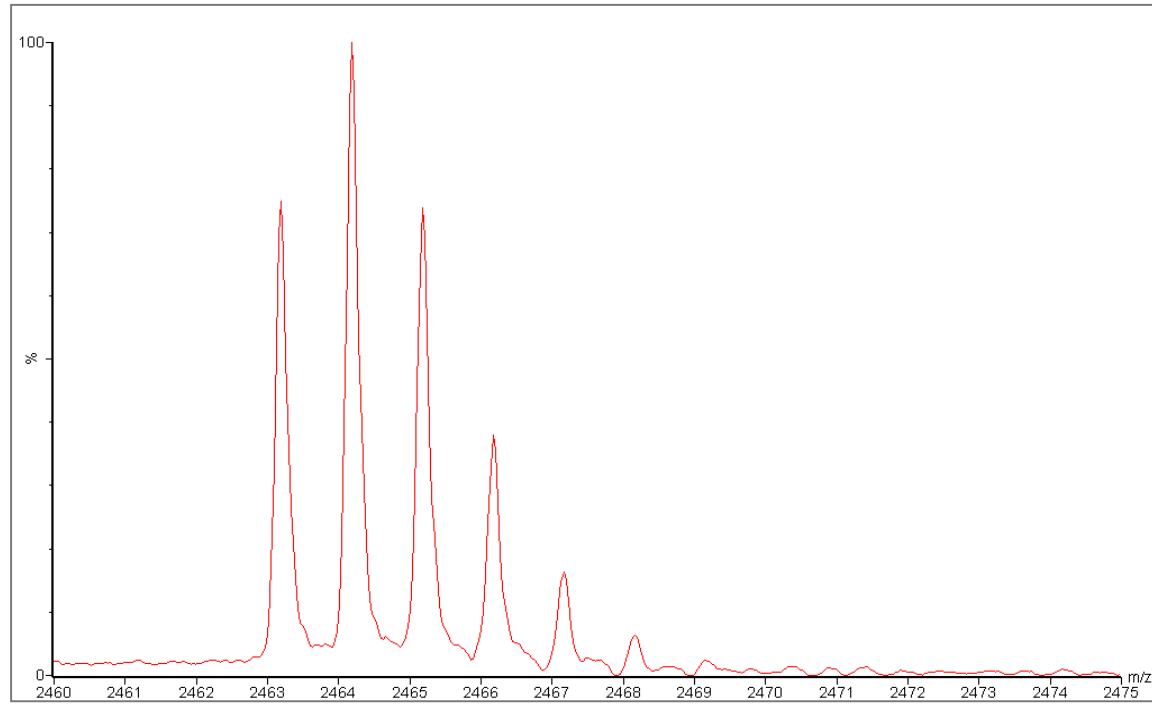


Figure 2. Example of resolution in reflectron mode (negative). Observed resolution $\approx 13,000$.

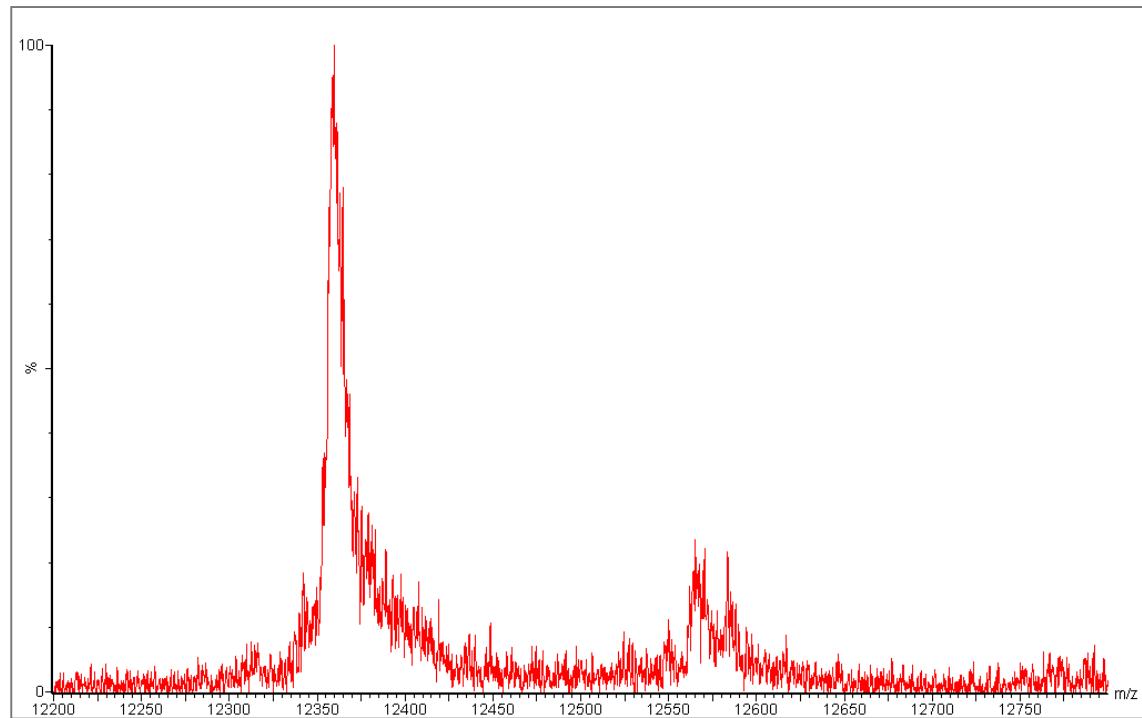


Figure 4. Example of resolution in linear mode (positive). Observed resolution ≈ 1350 .

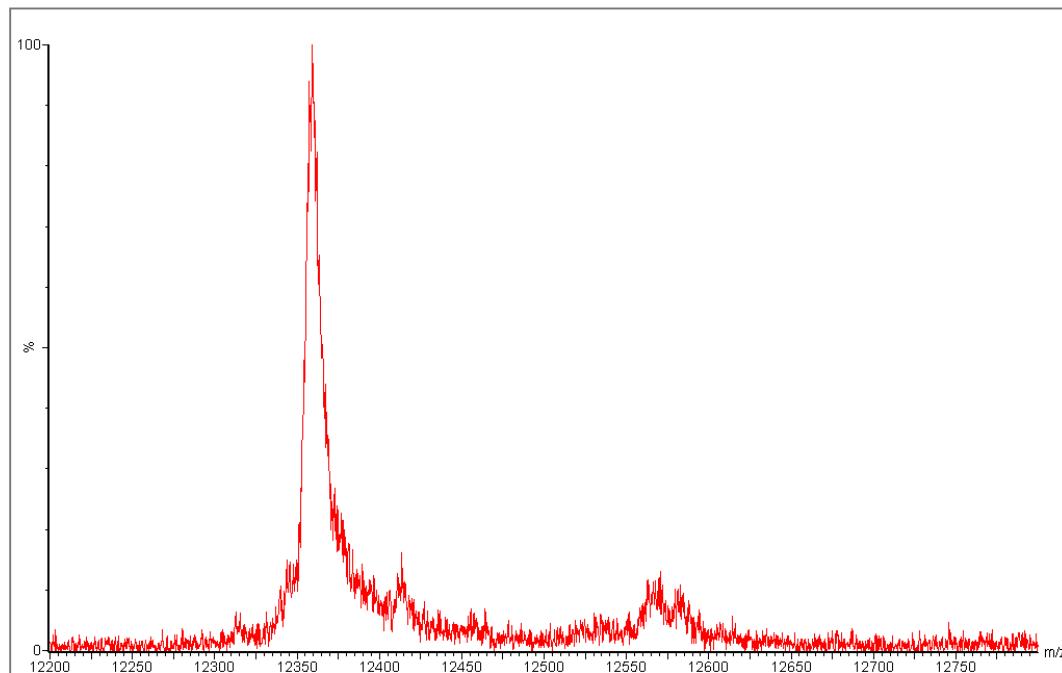


Figure 5. Example of resolution in linear mode (negative). Observed resolution ≈ 1150 .

CONCLUSION

- In this test the MALDI micro MX always surpassed the instrument specifications.
- In reflectron, positive ion mode a resolution of ca 16,000 was measured, 60 % better than the specified value of 10,000

REFERENCE

1. Tyler, A. N.; Clayton, E.; Green, B. N. *Anal. Chem.* **1996**, 68, 3561-3569.

WATERS CORPORATION
34 Maple St.
Milford, MA 01757 U.S.A.
T: 508 478 2000
F: 508 872 1990
www.waters.com

Waters

For Complete Confidence