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Applikationsbericht

An Evaluation of the MassLynx v4.1 AutoTune Wizard for the Development of MRM Methods

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This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief demonstrates compares the new AutoTune wizard to the manual tuning capabilities of an experienced analyst, and shows that the results generated by both methods are comparable.

Introduction

Creating multiple reaction monitoring (MRM) methods is an essential, yet labor-intensive part of developing sensitive and robust quantitative methodology on a tandem quadrupole LC-MS/MS system. Waters MassLynx v4.1 Software now features an integrated AutoTune Wizard with MS method development capabilities to make the calibration of the mass spectrometer, creation of appropriate tune files, and the creation of single ion recording (SIR) and MRM methods easier than ever for the analyst.

In this application brief, we compare results generated from utilizing the AutoTune wizard versus a manual tune performed by an experienced analyst for the creation of MRM methods involving ten compounds with a wide range of structural characteristics and ionization properties (Figure 1).

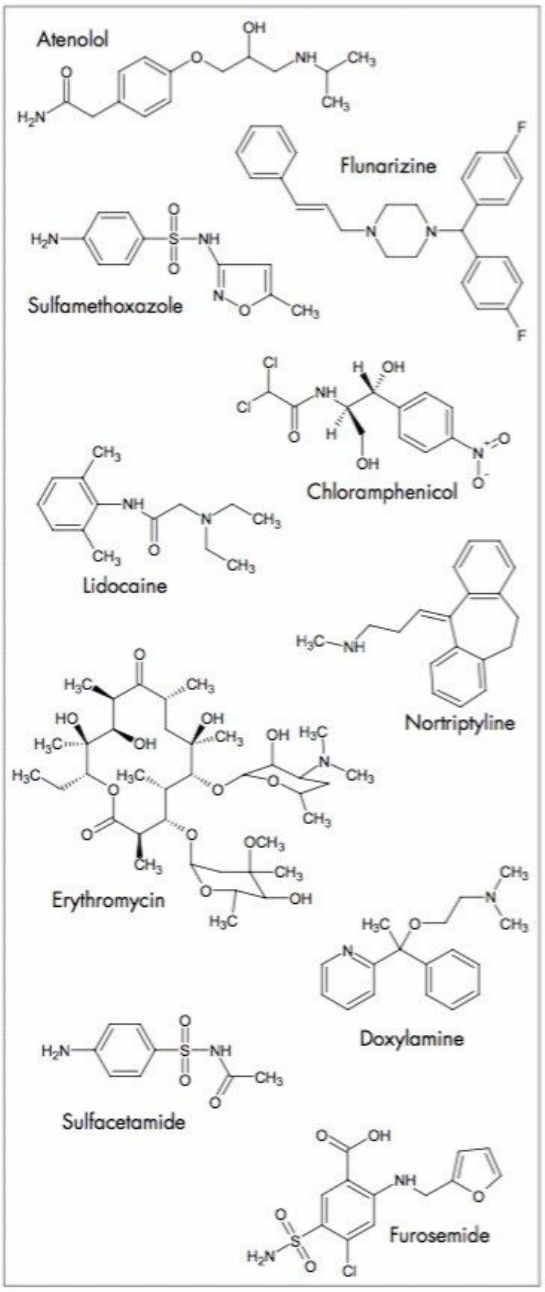

Figure 1. Structures of the ten test compounds.

Experimental

For both the AutoTune wizard and the manual tuning process, the LC flow was provided by an isocratic pump

at 600 µL/min using a 1:1 mixture of deionized water and HPLC-grade methanol as eluent. The tuning solutions of each compound were prepared at concentrations of approximately 200 ng/mL in methanol, then infused into the LC flow at 10 µL/min. MS/MS detection was facilitated by the use of a Quattro Premier XE Tandem Quadrupole Mass Spectrometer.

The MRM Developer was run as part of the AutoTune wizard to optimize the source parameters for the compound of interest, and to find the most intense product ion and optimum collision energy. It then automatically produced an MRM method and an AutoTune report to show the optimization data used for the method generation.

Results and Discussion

In Table 1 below, a comparison of the results generated by the Auto Tune Wizard and those produced by an experienced analyst are directly compared for all ten compounds under test. A good correlation between both result sets was observed.

Compound Name	Manual/Auto Tune	Parent Mass	Daughter Mass	Cone Voltage	Collision Energy	Ion Mode
Atenolol	Manual	267.20	190.15	35	24	Positive ESI
	AutoTune	267.23	190.10	35	25	Positive ESI
Flunarazine	Manual	405.15	203.10	25	21	Positive ESI
	AutoTune	405.23	203.10	25	24	Positive ESI
Sulfamethoxazole	Manual	254.05	156.10	25	21	Positive ESI
	AutoTune	254.08	156.00	25	21	Positive ESI
Lidocaine	Manual	235.20	86.30	25	23	Positive ESI
	AutoTune	235.25	86.40	25	25	Positive ESI
Chloramphenicol	Manual	321.05	152.00	30	22	Negative ESI
	AutoTune	320.99	152.00	30	23	Negative ESI
Erythromycin	Manual	734.45	158.20	30	42	Positive ESI
	AutoTune	734.49	158.20	30	43	Positive ESI
Nortyriptyline	Manual	264.20	91.30	30	27	Positive ESI
	AutoTune	264.23	91.30	30	30	Positive ESI
Sulfacetamide	Manual	215.10	156.10	20	13	Positive ESI
	AutoTune	215.17	156.10	20	16	Positive ESI
Doxylamine	Manual	271.20	182.15	20	19	Positive ESI
	AutoTune	271.20	182.10	20	19	Positive ESI
Furosemide	Manual	331.25	313.35	25	12	Positive ESI
	AutoTune	331.31	313.40	25	11	Positive ESI

Table 1. A comparison of AutoTune vs. manual tune results for all ten test compounds.

Conclusion

- The AutoTune wizard is now available as standard with MassLynx v4.1 for all quadrupole-based Waters MS Technologies.
- In this study, we have compared the new AutoTune wizard to the manual tuning capabilities of an experienced analyst, and have shown that the results generated by both methods are comparable.
- As well as the MRM Developer demonstrated in this work, the wizard also includes an SIR Developer and an Automatic Calibration tool.
- All of these MassLynx v4.1 features combine to bring new levels of ease-of-use and productivity for quadrupole MS applications, especially for inexperienced mass spectrometry users.

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MassLynx MS Software <https://www.waters.com/513662>

720001794, June 2006