The hybrid QQQ/LIT mass spectrometer has been shown to be an excellent tool for metabolite identification, primarily due to its ability to detect low abundant ions. The high quality data generated by these instruments allows for accurate metabolite quantitation. The sensitivity of the instrument is greatly increased by selecting for the most intense fragment ion from the lower energy spectrum. This approach is based on the observation that a higher ion fragment energy will result in the generation of more ions as a result of the collision cell fragmentation process.

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**MATERIALS AND METHODS**

**Introduction**

A 4000 Q TRAP® system (Applied Biosystems/MDS Sciex) was interfaced with Shimadzu LC-10AD vp autosamplers. Mobile phases used were Buffer A: H 2O + 0.1% v/v formic acid and Buffer B: Acetonitrile + 0.1% formic acid at a 40:60 ratio. The QQQ/LIT LCMS system was employed for the detection and identification of metabolites using a hybrid QQQ/LIT LCMS system.

**Methods and Conditions**

A script was written that allowed automatic generation of the complete methods used for metabolite identification. This script uses parameters determined to build precursor, parent ion, neutral loss, and MS2 scan ranges. All methods use 0.1% formic acid as the internal standard. The automatic method building script used the information generated in the optimization to build precursor (fragment 122 m/z) and parent compound methods for each ion. The automatic method building script used the information generated in the optimization to build precursor (fragment 122 m/z) and parent compound methods for each ion.

**Results**

The automatic method building script used the information generated in the optimization to build precursor (fragment 122 m/z) and parent compound methods for each ion. The automatic method building script used the information generated in the optimization to build precursor (fragment 122 m/z) and parent compound methods for each ion.

**Conclusions**

An automated metabolite identification software script proved useful in generating appropriate QQQ/LIT LCMS methods. The methods generated using the new method builder software, Metabuilder, yielded data equivalent to data that was acquired using operator generated QQQ/LIT LCMS methods. The methods generated using the new method builder software, Metabuilder, yielded data equivalent to data that was acquired using operator generated QQQ/LIT LCMS methods.

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**References**