Application of the X500R QTOF system in new psychoactive substances in electronic cigarettes

Mu Pengqian[1], Zhang Xiaogang[1], Yang Zong[1], Liu Bingjie[1] and Guo Lihai[1] , Neil Walsh[2]
1.SCIEX Asia Pacific Application Support Center, Shanghai, China 2.SCIEX USA

INTRODUCTION

The main components of ordinary electronic cigarettes are water, propylene glycol, glycerin, nicotine and flavoring agents, but the components of some electronic cigarettes have been illegally mixed with synthetic cannabinoids and new psychoactive substances (NPS). This special electronic cigarette oil can be consumed using ordinary electronic cigarette sets, with low threshold and high concealment. Tobacco oil that contains high-purity marijuana extract and synthetic cannabinoids can be more addictive than cannabis. Therefore, it is important to rapidly and sensitively evaluate the presence of NPS in electronic cigarettes. Accurate mass spectrometry systems have been shown to be powerful for qualitative analysis. In this work, an efficient method for the detection of NPS in electronic cigarette products was developed using liquid chromatography-accurate mass spectrometry.

METHODS

Sample preparation: An appropriate amount of ground solid or liquid sample was placed into a volumetric flask and dissolved with methanol. The volume was then adjusted, and the sample was extracted by ultrasonic mixing. After centrifugation, the sample was injected onto the X500R QTOF system coupled with an ExionLC system.

HPLC conditions: An SCIEX ExionLC AC system was used for analytical separation using a Phenomenex C18 column (2.6 µm, 2.1 × 100 mm). The compositions of the mobile phases were 0.1% formic acid in water and methanol. The flow rate was 0.4 mL/min with a column temperature of 40°C. The injection volume was 2 µL.

MS/MS conditions and data processing: TOF MS data and MS/MS data were acquired in 1 injection using the information-dependent acquisition (IDA) scan mode with dynamic background subtraction (DBS) enabled. The MS source conditions were optimized as follows: curtain gas (CUR), 30 psi; collision gas (CAD), medium; nebulizing gas (GS1), 55 psi; heater gas (GS2), 55 psi; ion spray voltage (IS), 5500V in positive ion mode; and source temperature, 550°C. Other mass spectrometry parameters used are presented in Table 1. Data processing was performed using SCIEX OS software, version 2.1.

To receive a copy of this poster:

- Scan the code with your phone camera
- Complete the form

Table 1. Mass spectrometry parameters.

Mass spectrometry parameters	Settings
TOF MS	*100-1000 Da*
TOF MS/MS	*50-1000 Da*
Dynamic background subtraction	*On*
Candidate MS/MS per cycle	*12*

RESULTS

In this study, more than 400 new psychoactive substances were screened for in 2 electronic cigarette products on the market. Sample preparation and LC-MS parameters were optimized to develop a final screening method. After acquisition, sample data and the compound screening list were imported into SCIEX OS software. To confirm compound identity, the SCIEX OS software automatically compared the precursor ion mass error, precursor isotope ratio, as well as compared the MS/MS fragmentation spectra against as library database. New psychoactive substances 4-CEC and 4-F-α-PVP were detected in the sample. The mass errors were all within 1 ppm, indicating that the instrument had good mass accuracy and stability. The MS/MS spectrum match to the database was greater than 96/100 points (Figure 1).

NPS are constantly changing as different compounds emerge in the market. For this reason, the existing screening list may be insufficient to detect all NPS in the samples. Therefore, non-targeted screening to find compounds that differ between the samples and blank controls is essential for NPS screening. Once the blank control and samples were imported into SCIEX OS software, the software automatically compared the samples to identify differences between them. The SCIEX OS software then linked automatically to the ChemSpider website to search for possible compound structures for the unknown compounds detected in samples (Figure 2). These compound structures were then matched with MS/MS spectra to identify possible structures. When confirming new derivatives, ChemDraw software was used to draw the hypothesized structural formula, which was then imported into SCIEX OS software. The Fragments pane function of the software was used to analyze the fragments of the compound to confirm the accuracy of the structure (Figure 3).

This work highlights the full method for non-targeted screening using accurate mass LC-MS and SCIEX OS software.

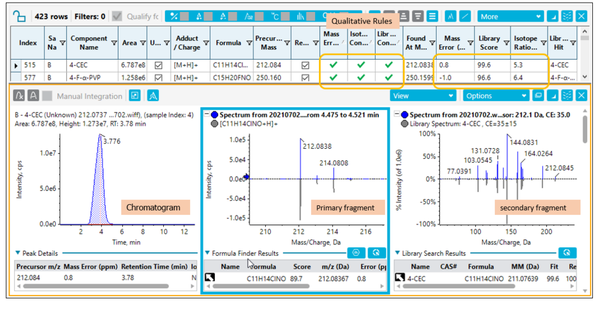

Figure 1. Qualitative of 4-CEC and 4-F-α-PVP.

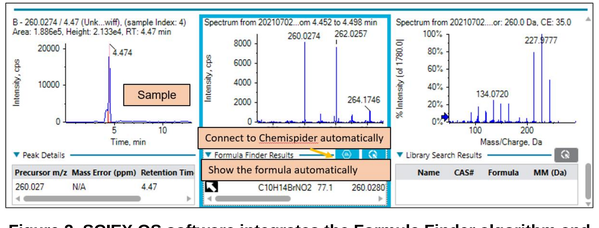

Figure 2. SCIEX OS software integrates the Formula Finder algorithm and ChemSpider for novel NPS identification.

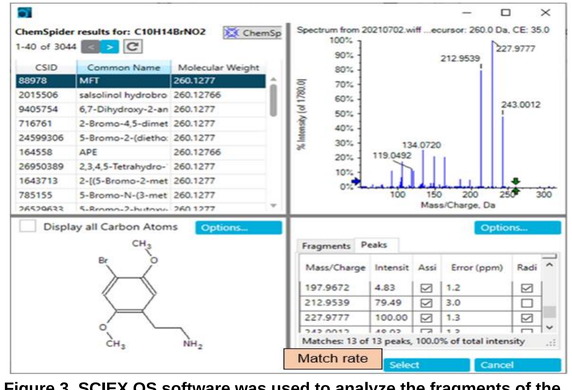

Figure 3. SCIEX OS software was used to analyze the fragments of the compound to confirm the accuracy of the structure.

CONCLUSIONS

The X500R QTOF system has an ultra-fast scanning speed (100 Hz) that allows a single injection to achieve both high-quality precursor and product ion scans. It combines the rich high-resolution NPS MS/MS spectra library and ChemSpider database to quickly and easily identify unknown features. The powerful SCIEX OS software provides easy-to-use tools to facilitate the discovery of new NPS and also to obtain structural analysis. In conclusion, the X500R QTOF system provides high-quality hardware and software for the detection of new psychoactive substances and provides powerful software workflows for the rapid screening and detection of NPS.

TRADEMARKS/LICENSING