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Electrospray-ionization MS/MS library of drugs as database for method development and drug identification

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Abstract

An ESI MS/MS library of 800 compounds has been developed and a collection of data is now available for Analyst 1.4 and higher. Compounds include forensically important drugs, such as illegal drugs, some deuterated analogues, hypnotics, amphetamines, benzodiazepines, neuroleptics, antidepressants and many others. For setting up the library of product ion spectra, 20–200 ng of the compounds have been injected either by flow injection or via a short LC-column, the precursor ions were chosen from the Q1 scan spectra, and product ion spectra were generated by CID in the collision cell using three different collision energies (20, 35 and 50 eV). Three spectra of each compound have been collected and compound names, CAS numbers, formulas and molecular weights have been added in the database, which has been generated by the Analyst software. The library can be used for compound identification during general unknown screening analysis by combination of Q1 scan techniques and subsequent MS/MS analysis in a second analytical run. Quantitative procedures for multi drug analysis using Multiple Reaction Monitoring can be established by selection of product ions and suitable collision energies from the library. For publication of the spectra, PDF-files have been generated and can be viewed on-line as supplementary data or from the website in alphabetical order: http://www.uniklinik-freiburg.de/rechtsmedizin/live/forschung/projekte/lcmsms/ms2-2005-index.html [1] (supplementary data, should be made available via ELSEVIER-WEBSITE or via http://www.uniklinik-freiburg.de/i/rme/de/pix/ms2-2005-index.html).

Keywords: Electrospray-ionization; LC–MS/MS library of drugs; Library searching; General unknown analysis; Target analysis; Compound identification

1. Introduction

In recent years liquid chromatography/mass spectrometry (LC/MS) has developed to a complementary method for gas chromatography/mass spectrometry (GC/MS) and liquid chromatography/diode array detector (LC/DAD) for general unknown screening (GUS) [2,3] especially for thermal unstable and polar compounds or substances without or with insufficient UV absorbance. Mass spectral libraries, generated by electrospray ionisation (ESI) or atmospheric pressure chemical ionisation (APCI) are available including spectra of drugs, pesticides and explosives obtained by ''in source'' collision induced dissociation (in source CID) resulting in searchable spectra [4–6]. However, in case of co-eluting substances or matrix components from extracts of biological material, identification of analytes may be difficult due to impure mass spectra and decreased fit values after library searches.

Triple-quadrupole mass spectrometers with CID in the collision cell provide mass spectra, which are practically free of background by selection of the precursor in the Q1, and several MS/MS libraries have been developed using triple-quadrupole mass spectrometers [7–9]. With these libraries substances detected by a GUS with LC (single stage)–MS can be identified by recording their product ion spectra in a second analysis [10] or in the same LC run applying an information dependent acquisition (IDA) either with a triple-quadrupole mass spectrometer equipped with a linear ion trap [11] or with a Q-TOF instrument [12]. Acquired MS/MS spectra can then be identified if present in the MS/MS library.

Conventional ion traps also have been used to establish MS/MS and MS^3 spectral libraries to perform GUS with IDA, which allows – like IDA with linear ion traps – detection and identification of substances in one LC analysis [13,14].

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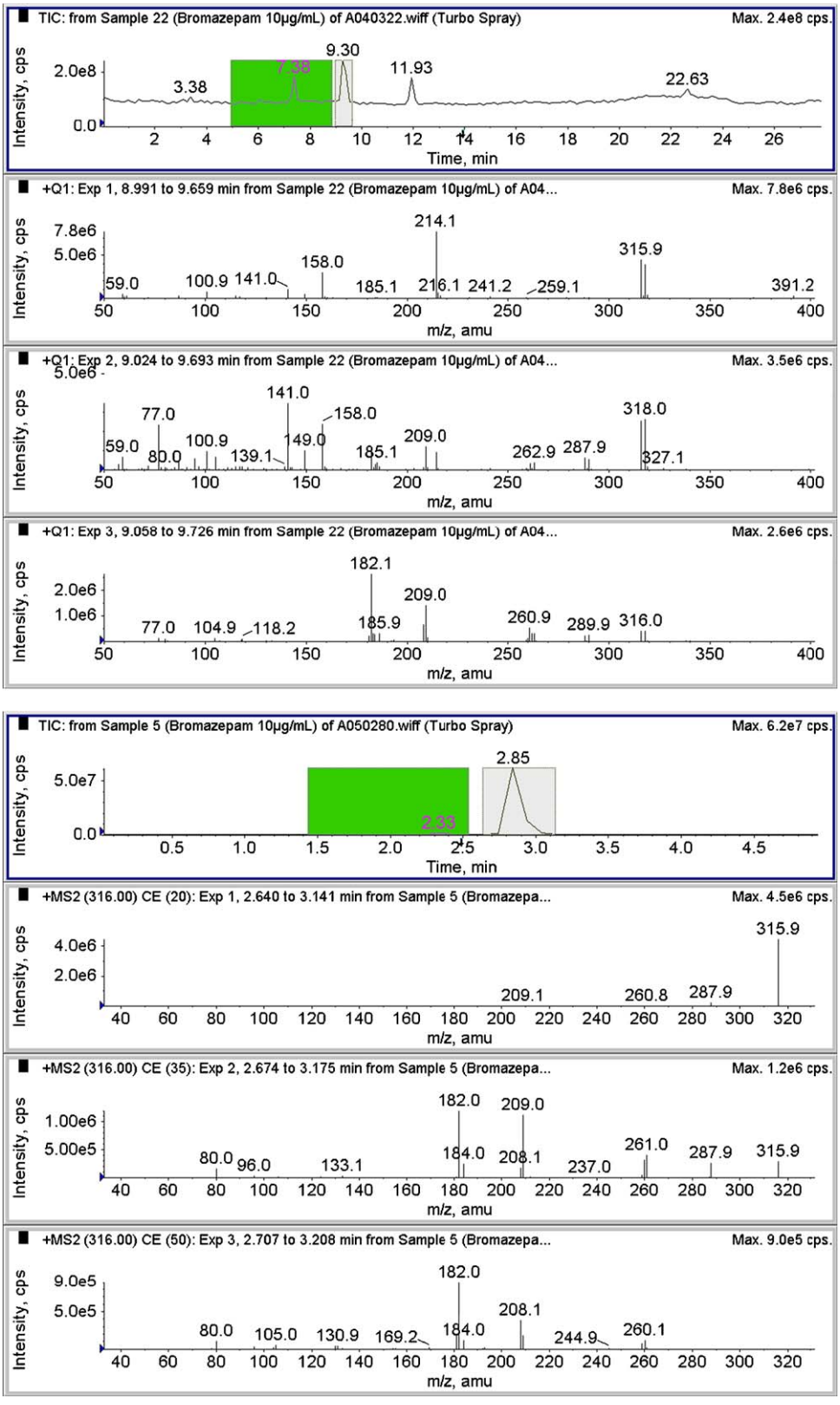

Fig. 1. LC–MS analysis (total ion chromatogram and spectra) for the identification of the precursor ion of bromazepam at 20, 50 and 80 V declustering potential in single-quadrupole scan mode (top) and LC–MS/MS analysis to obtain product ion spectra of bromazepam at 20, 35 and 50 eV collision energy, respectively (bottom).