Evaluation of sensitivity enhancement using a high-temperature ESI-source for various compounds of forensic interest

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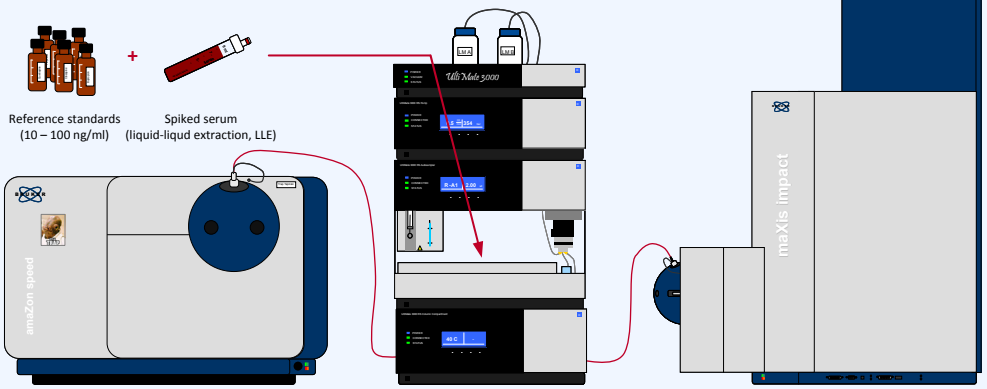
INTRODUCTION

Sensitivity is of major importance for most MS applications especially when it comes to trace analysis in forensic toxicology. The enhancement of MS intensity can lower the detection limits in threshold triggered screening methods employing full scan capable instrumentation like ion trap and TOF MS instruments. In this study the impact of a new high-temperature ESI source on the ionization efficiency of analytes of interest for forensic toxicology (synthetic cannabinoids, designer stimulants, psychotropics, benzodiazepines, basic drugs, alcohol consumption markers…) has been investigated.

METHODS



Evaluation experiments were carried out on an amaZon speed™ ion trap and a maXis impact™ Q-TOF mass spectrometer, each equipped with an ionBooster™ (IB) and standard ESI-source. Data was acquired in UltraScan mode (ion trap) and fullscan mode (Q-TOF), respectively.

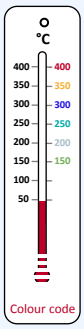
Preliminary data showed, that the vaporizer gas temperature (IB) has a greater influence on the ionization efficiency as dry gas temperature and sheath gas flow.

The latter were optimized according to an LC flow of 0.5 ml/min and kept constant while for each analyte the vaporizer gas temperature was subsequently increased (150 - 400 °C).

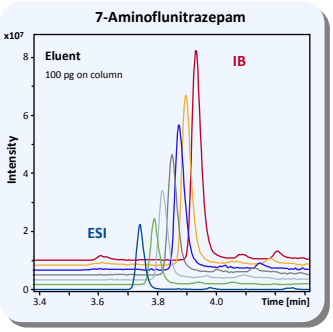
ionBooster™
dry gas temp.: 200°C
sheath gas flow: 150 l/h

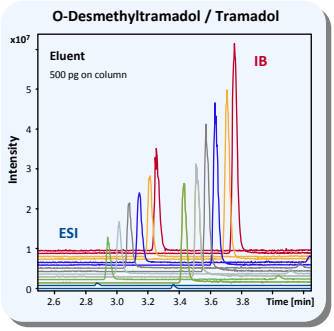
ESI Source
Dry temp.: 320°C
dry gas: 10 l/min

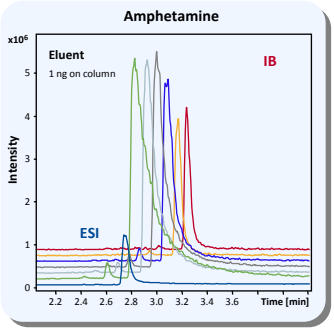
ionBooster vaporizer gas temperature

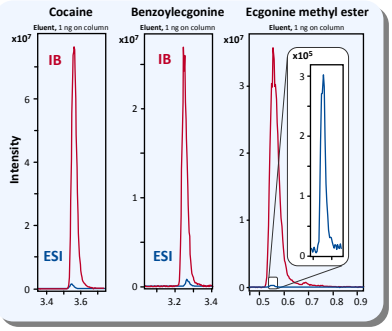


RESULTS

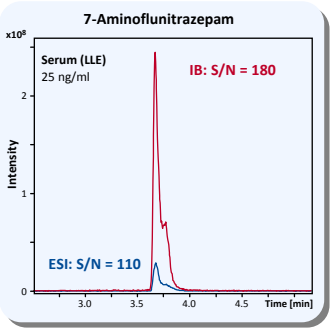


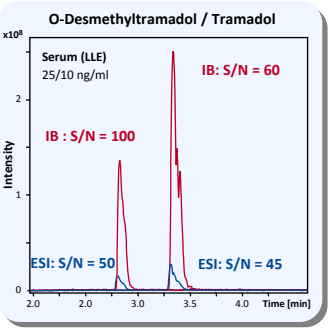


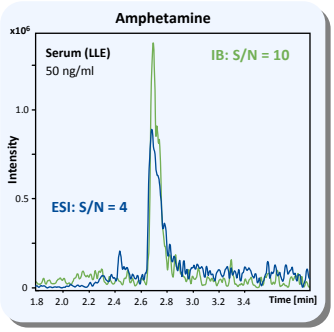


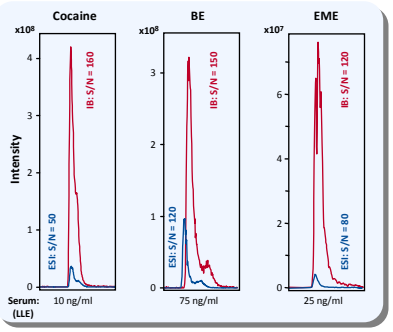


This study revealed a significant intensity gain for the majority of compounds investigated. The vaporizer temperature has a great influence on the degree of enhancement/impairment of the respective signal intensity and should be chosen with care. The signal intensity is up to tenfold higher than with conventional ESI for most of the evaluated compounds. The individual sensitivity improvement though, varies due to the compounds different chemical characteristics, ionization behaviour and thermal properties, but none of the analytes investigated showed a decrease of intensity with IB. No notably different in-source-fragmentation or adduct formation was found. Also most matrix-related signals experienced less enhancement than the analytes, leading to improved signal-to-noise ratios.









Synthethic cannabinoids: In average, fivefold higher signal intensities were observed in eluent. Applying a vaporizer gas temperature of 350 °C as a compromise for all incorporated analytes, still lead to a signal enhancement by a factor of at least two compared to ESI. In serum, this enhancement enables the detection of compounds not detected when using conventional ESI[1] and detection limits in the range of 0.1 to 0.5 ng/mL.

Psychotropic drugs: The eluent data of more than 50 psychotropic drugs showed signal enhancement of factor 3 to factor 20 when using a vaporizer gas temperature of 400 °C. Consequently, the ionBooster was implemented during method development of a screening method for the detection of psychotropic drugs in biological matrices[2].

CONCLUSIONS

The ionBooster leads to higher signal intensities for all compounds investigated within this study. The observed signal enhancement could make threshold triggered screening solutions applicable to samples where only little material is available and/or low analyte concentrations are expected or traditionally recognized (e.g. hair, oral fluid). This preliminary data also reveals, that - aside from pure signal enhancement - the signal-to-noise ratio in serum can be increased. Hence, for the development of LC-MS methods involving analytes investigated in this study, the usage of high-temperature ESI should be considered.

REFERENCES

[1] Huppertz et al.: 'Trapping Spice': Detection of currently 46 synthetic cannabinoids using an automated LC-MS^n screening approach (PE$_{19}$), **51st TIAFT Meeting, Funchal, Madeira, 2013**

[2] Kempf et al.: 'Psychotropics caught in a trap' - Adopting a screening approach to specific needs (PE$_{18}$), **51st TIAFT Meeting, Funchal, Madeira, 2013**