Comparison between Toxtyper™ and LC-Quadrupole-Time-of-Flight-MS in post-mortem toxicology

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Background
The Toxtyper™ (Bruker; TT) and the LC-QTOF-MS (Waters; Xevo G2-S Quadrupole Time-of-Flight Mass Spectrometer) are both powerful screening techniques for post-mortem toxicology. Both modalities have detections based on mass-to-charge ratio but differ with regard to the type of mass detection, sensitivities, and toxicology libraries. We aimed to evaluate the accordance in post-mortem toxicology results after screening of samples both by TT and LC-QTOF-MS.

Methods
Seventy-one whole blood samples from post-mortal cases were analyzed with both TT and the LC-QTOF-MS in two different laboratories. The frequency of identical and deviating qualitative results was calculated.

Results
The 71 samples gave 207 positive results with the TT and 249 with the LC-QTOF-MS. Fifty-three (75%) of these samples led to an identical interpretation, ten (14%) samples led to a possible and another eight (11%) to a definite different interpretation. In 17 (24%) of the 71 cases the TT did not find any substances, and in five of these cases the LC-QTOF-MS did find one or more compound(s), e.g. amiodarone, clindamycin and atorvastatin. The LC-QTOF-MS did not find any compounds in fourteen of the cases (20%) while the TT could detect one or more compound(s) in two of them, e.g. lisinopril and tranexamic acid.
In three of eight cases with a definite different interpretation, the LC-QTOF-MS reported amiodarone (including its metabolite), and found in other cases a.o. ocfentanil and m-trifluorophenylpiperazin (TFMPP). In three other cases with a definite different interpretation, the TT reported tranexamic acid (once) and ethylglucuronide (twice).

Conclusions
In 14% of the cases the TT and LC-QTOF-MS led to a possible and in 11% to a definite different interpretation. If compounds are among others not part of the library, are not recovered after sample preparation or have difficulties in ionization, differences in outcome can be expected. These results call for a general method of screening based on the lower limit of detection but also on a semi-quantitative value in the upper therapeutic to toxic range of drugs that are regularly used or abused to improve forensic and clinical interpretation.

Key Words
Toxtyper™
LC-Quadrupole-Time-of-flight-MS
Post-mortem toxicology