BUILDING A FORENSIC GC-MS/MS MRM DATABASE

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BACKGROUND
• An ever growing and changing toxicant landscape makes it impossible to obtain analytical standards for every (novel) chemical.
• Labs are looking for robust & pragmatic methods for confirmation of the presence of a toxicant.
• Gas chromatography coupled to mass spectrometry (GC-MS) is an easily optimizable technique available in many forensic labs, that generates uniform & comparable results between instruments and labs.
• The use of tandem mass spectrometry (MS/MS) can improve selectivity & sensitivity.

OBJECTIVES
• Building a database of readily available MRM transitions for (forensic) toxicologically relevant chemicals that are compatible with GC.
• Developing a workflow for practical and straightforward addition of more (new) toxicants.

METHODOLOGY
• Instrument: Agilent 7890B GC coupled to a 7000D triple quadrupole MS
• Stationary phase: Agilent DB-5MS capillary column (30 m x 0.25 mm x 0.25 µm)
• Carrier gas: He
• Injection: pulsed splitless mode – V = 2 µL
• Retention time locking to cocaine to 12.26 min
• Electron impact ionisation: source temperature = 230 °C, electron energy = 70 eV

MRM CURATION WORKFLOW

MRM Curation Workflow Diagram

APPLICATION
• Proof of concept: application to archived post-mortem blood samples (n = 25)
• Comparison full scan only with MRM
• All compounds found with MRM approach, not with full scan only
• E.g. fentanyl in therapeutic concentration range (1.7 ng/mL)

CONCLUSIONS
• A database of readily available MRM transitions for relevant toxicants was established and successfully applied to authentic samples.
• The developed MRM database can be tested and used with any GC-MS/MS instrument, simplifying the development of screening and quantitation methods in forensic labs.
• The developed MRM curation workflow showed the potential to continuously add new chemicals to the database in a uniform and practical way.

FUTURE PERSPECTIVES
• Addition of more novel toxicants & their metabolites to the database, sharing library and crowd-sourcing.
• Continued authentic samples analyses: tablets, powders, urine, vitreous humour, tissues (e.g. kidney, liver), ...
• Implementation in routine screening methods.

References