

Methylmethcathinone (MMC) isomer identification : brain teaser illustrated by a case report

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BACKGROUND

CLINICAL CONTEXT

Patient treated for withdrawal from an admitted addiction to 2-MMC → test his blood to confirm the abstinence

Considering the results

We asked for the consumed powder



UNRELATED CASES

FORENSIC CONTEXT

5 unrelated powder samples for identification



METHODS

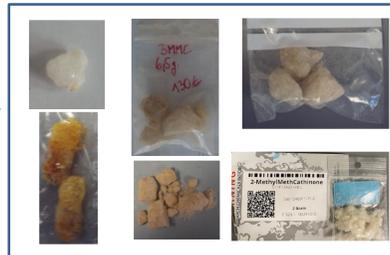
Liquid-liquid extraction

HPLC-DAD (Waters)
Alliance 2695 + PDA 2996
Symmetry C8 - PO₄ Buffer - ACN

UHPLC-TOF-MS (Sciex)
Eksigent LC 100 XL + TripleTOF 4600
Kinetex C18 - NH₄HCOO/ACN/MeOH



Dilution in mobile phase



Dilution in CHCl₃
GC-MS (Agilent)

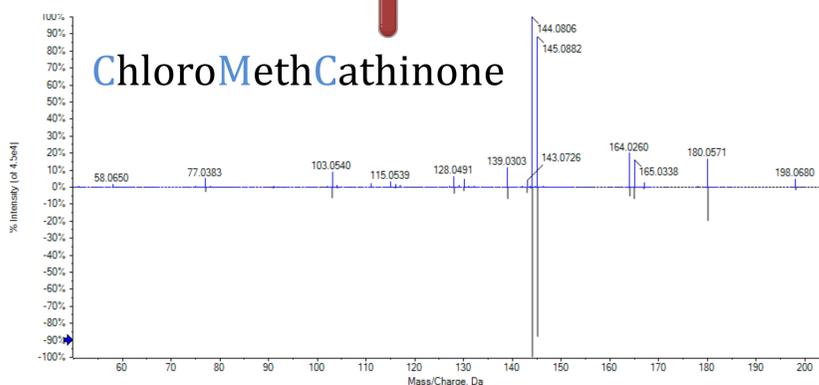


Dilution in KBr
Infrared Spectroscopy (Bruker)

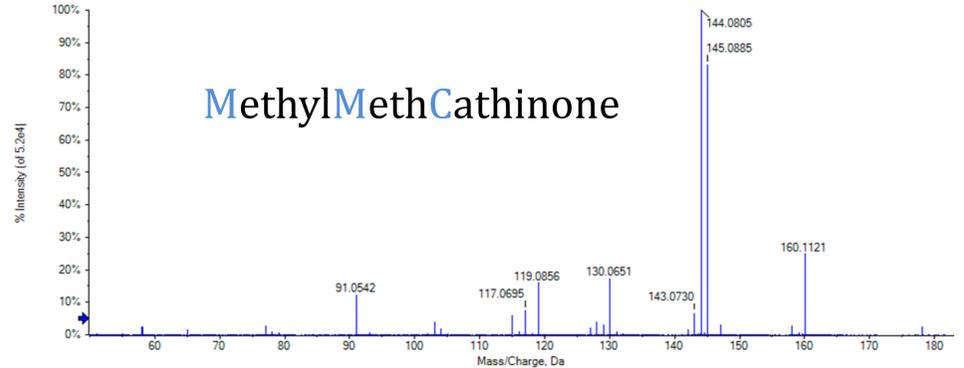


RESULTS & DISCUSSION

Patient's blood



Patient's powder



The product consumed before the blood test came from a ≠ batch

Is it possible to distinguish between the MMC isomers without reference standards?

(initially, only 4-MMC in the lab)

With UHPLC-TOF-MS and GC-MS: NO: 2-,3-,4-MMC share the same retention time and MS spectrum

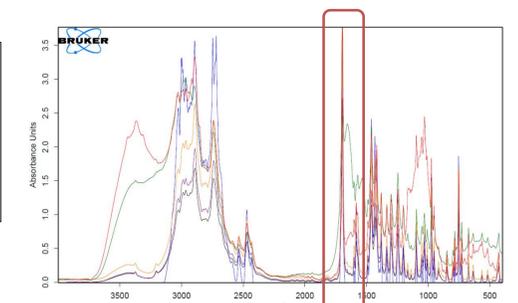
With HPLC-DAD and Infrared Spectroscopy: YES but our 6 powders share the same retention time, UV spectrum, and IR spectrum (including those labeled 2- and 3-MMC)

UV spectrum [1]:

- 4-MMC is very different
- small difference between 2- and 3-MMC

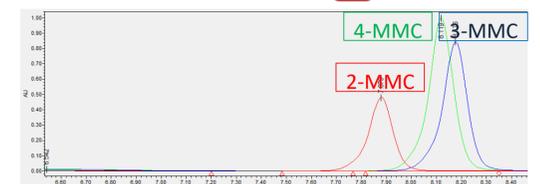
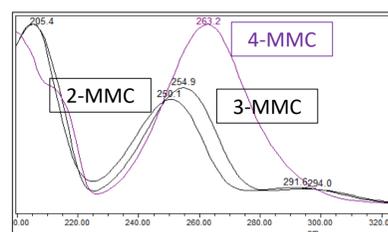
IR spectrum:

The carbonyl C=O stretching band for 3-MMC and 4-MMC are both at 1685 cm⁻¹ but 2-MMC has the carbonyl band at 1696 cm⁻¹



→ The 6 powders are identified as 2-MMC

After reception of reference standards



39%

41%

80%

82%

84%

85%

CONCLUSION

One NPS can be sold for another. The ability to distinguish between NPS isomers requires the use of analytical reference standards and/or additional analytical methods. HPLC-DAD is still very useful!