

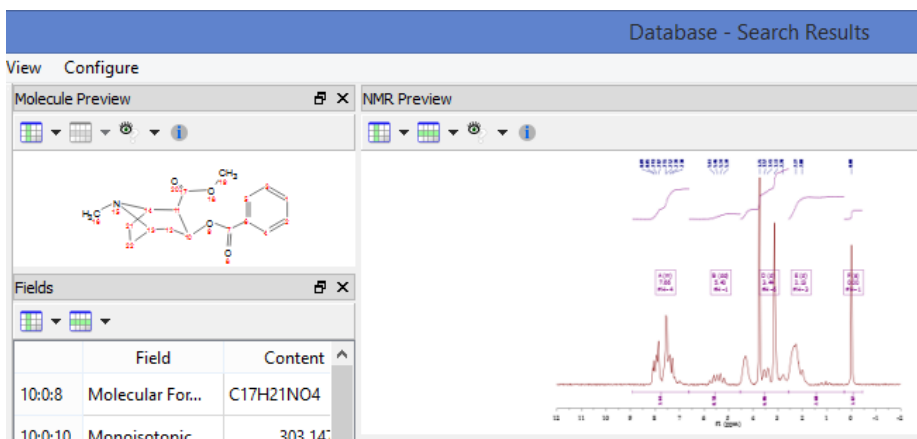
Forensics

Forensic scientists working with drug enforcement agencies all over the world are faced with the same questions - **What is this drug? How pure is it? How was it made?**

These scientists are presented with a wide range of drug samples, from products or precursors seized at border control to clandestine lab busts, and require a quick and reliable solution that will give specific identification and can also be used quantitatively. It has been recognized that NMR would be an invaluable technique for this purpose, however the costs and maintenance of high field NMR has limited its use. The Magritek Spinsolve benchtop NMR spectrometer is the ideal solution for forensics due to its small footprint, simple sample preparation and superior performance.

What is this drug?

The benefit of using NMR for drug identification is that it gives a specific fingerprint for each compound. A database can be used to quickly identify known drugs or that something is a new analogue. Structural elucidation of new drugs can be achieved using the multinuclear and 2D capability of Spinsolve.

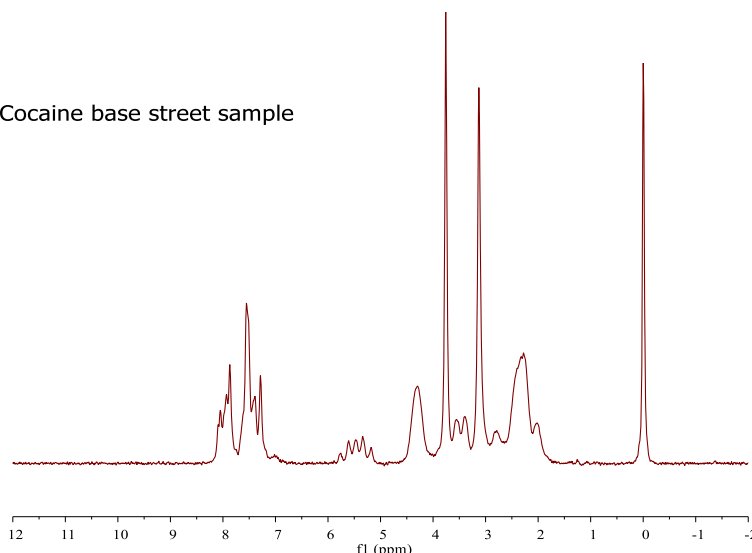


Field	Content
10:0:8 Molecular For...	C17H21NO4
10:0:10 Monoisotopic ...	303.14

Record	Item Type	Item Number	Search Score
2	mndb://...	NMR Sp... 1	500
7	mndb://...	NMR Sp... 1	500
11	mndb://...	NMR Sp... 1	500
16	mndb://...	NMR Sp... 1	772
21	mndb://...	NMR Sp... 1	533

Cocaine base certified reference material

Cocaine base street sample

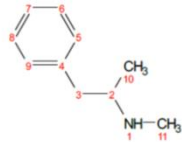


How pure is it?

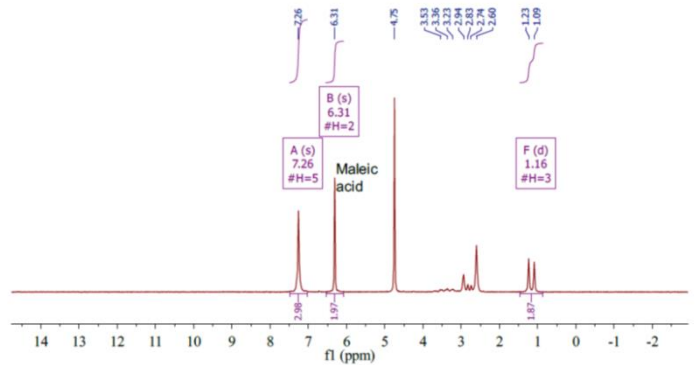
NMR spectroscopy is inherently quantitative, therefore there is no need for timely and expensive calibration.



1D-1H-"StandardScan"
Methamphetamine in D2O + Maleic acid internal std



Molecular mass 149.24 g·mol⁻¹
Maleic acid = 35.98 mg/ml in D2O

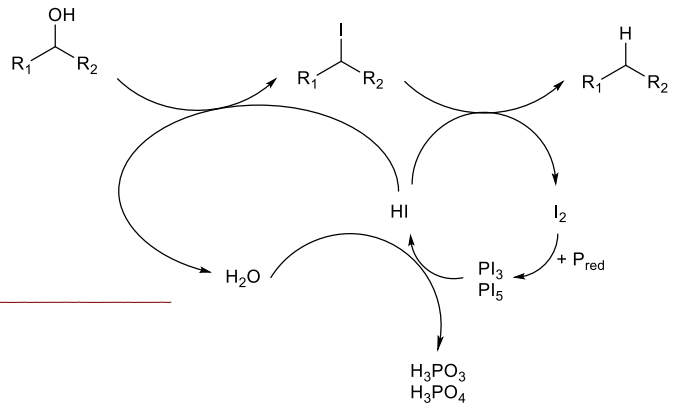
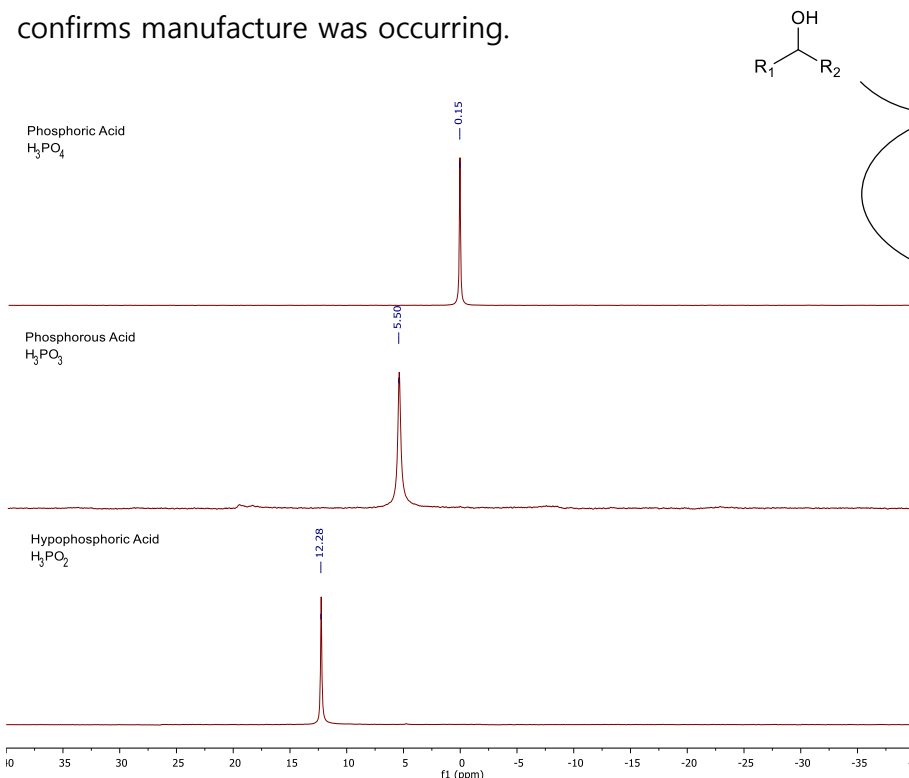


Parameter	Value
1 Data File Name	C:/Projects/sample1
2 Spectrometer	Magritek Spinolve
3 Number of Scans	4
4 Acquisition Date	2015-09-23T12:42:31.889
5 Total acquisition time (min)	1
6 Nucleus	1H

Multiplet
A(s) 5 7.49, 7.0351, 7.442
F(d) 3 1.46, 0.8655, 2.459
Purity Average: 53.1
RMSE%: 3.40
Assuming sample weight: 50.0000 mg, and mol weight: 149.2328
Using Reference Compound: Maleic Acid
(Compound: 0, Solvent: 0, 35.9800 mg, 99.9500% purity, Mol Weight=116.0700)
Parameters:
Multiplet Selection Method: Minimum RMSE
Integration Method: Sum with Integration Factor: 12

How was it made?

This can be difficult to determine using other methods, but with NMR it is straight forward. Products, starting materials and by-products can be identified and quantified. For example, the synthesis of methamphetamine often involves the reduction of ephedrine with red phosphorus and iodine. The phosphorus acids produced in the synthesis can be used to estimate how far through the synthesis the process was before being seized and on what scale it was being produced. The presence of phosphorus acids and methamphetamine confirms manufacture was occurring.

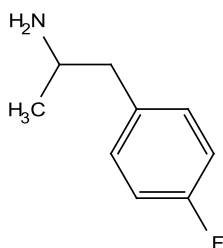


Multiple Nuclei

Spinsolve is capable of measuring a variety of different nuclei including ^1H , ^{19}F , ^{31}P and ^{13}C that can add to the investigation.

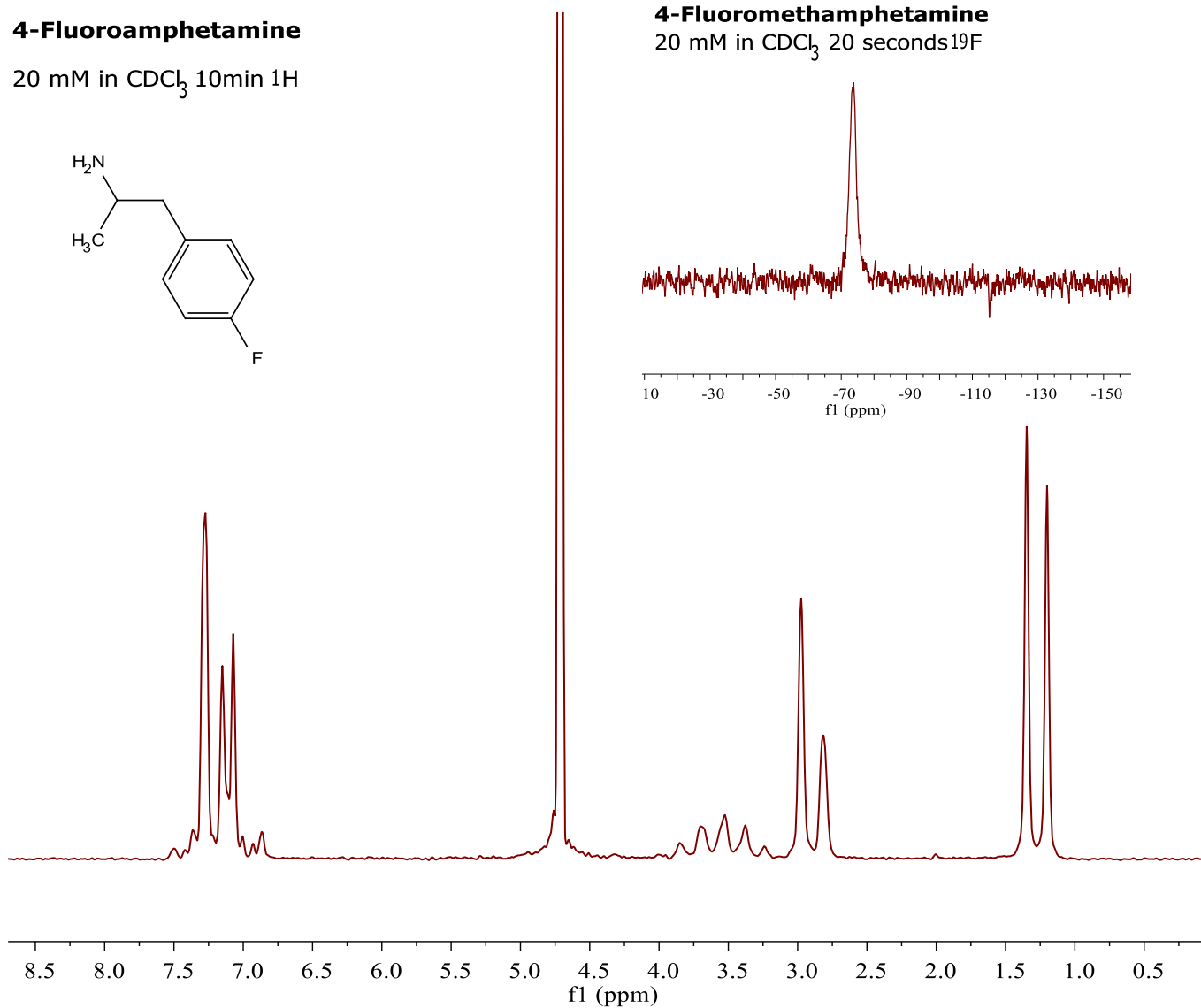
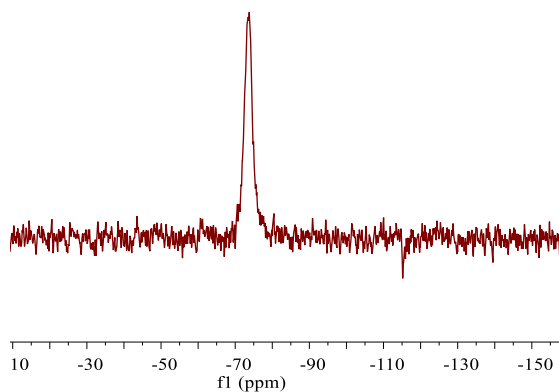
4-Fluoroamphetamine

20 mM in CDCl_3 10min ^1H



4-Fluoromethamphetamine

20 mM in CDCl_3 20 seconds ^{19}F

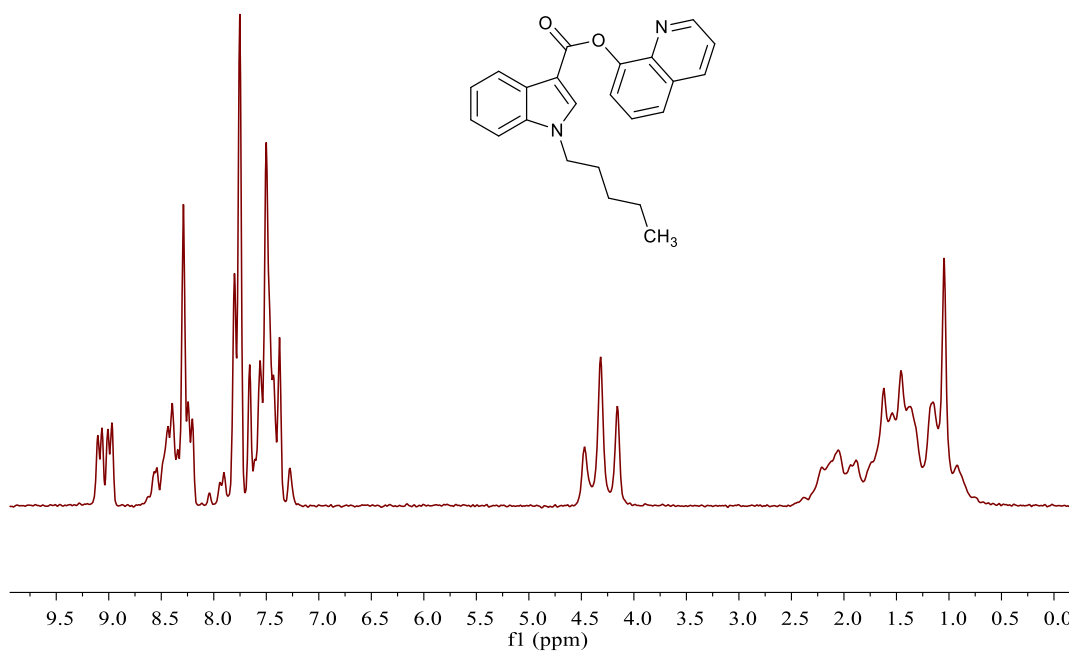


Related Compounds

Due to the specificity of NMR, Spinsolve can distinguish related compounds such as these synthetic cannabinoids.

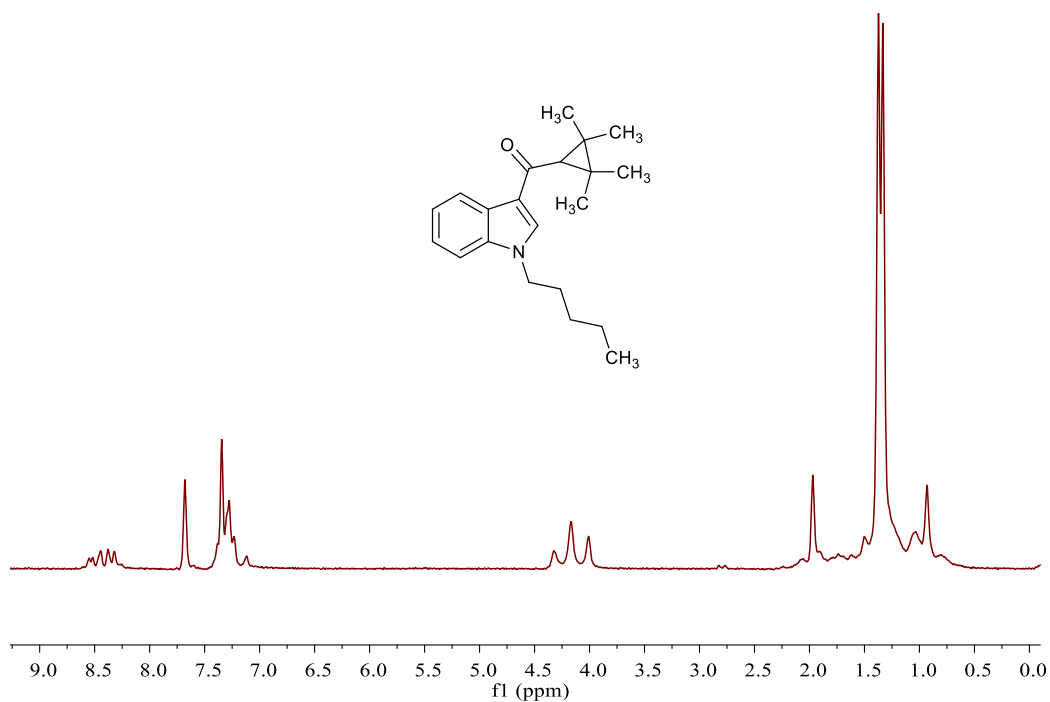
PB-22

100 mM in CDCl₃ 1H 10min

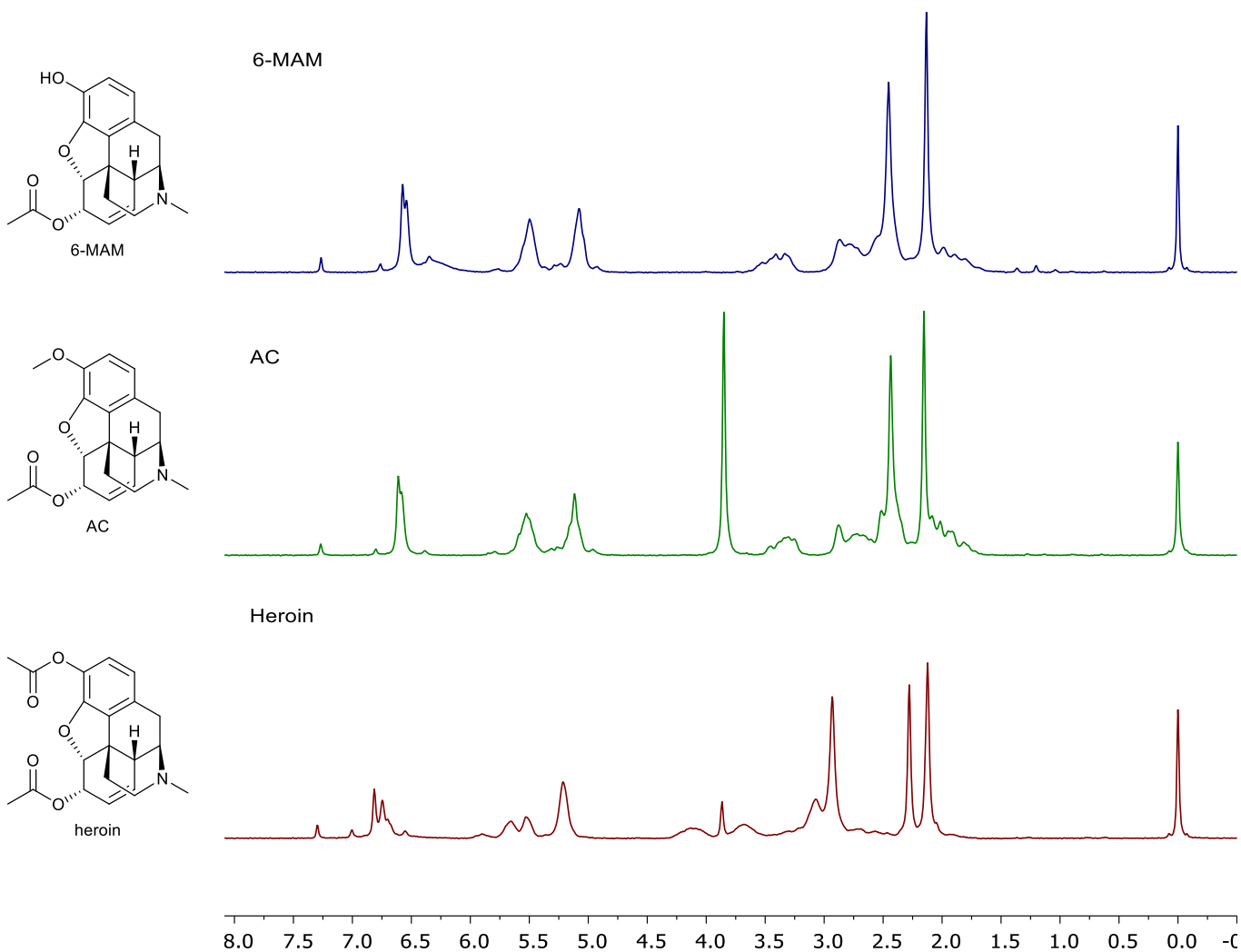


UR-144

100 mM in CDCl₃ 1H 10min



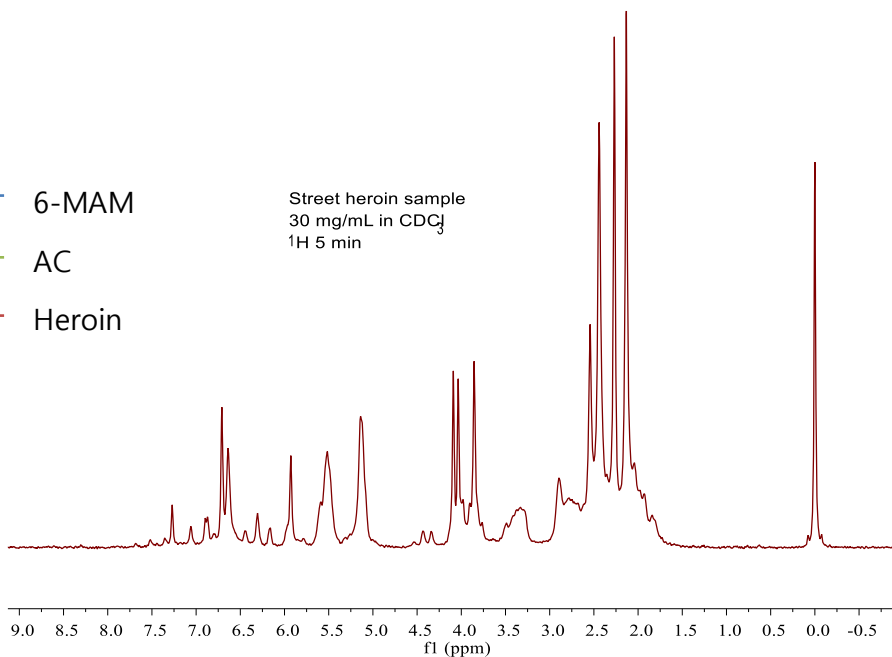
The degradation or by-products found in heroin can be distinguished and identified in a real sample.



Record	Item Type	Search Score
11	mndb://...	652
16	mndb://...	739
21	mndb://...	833

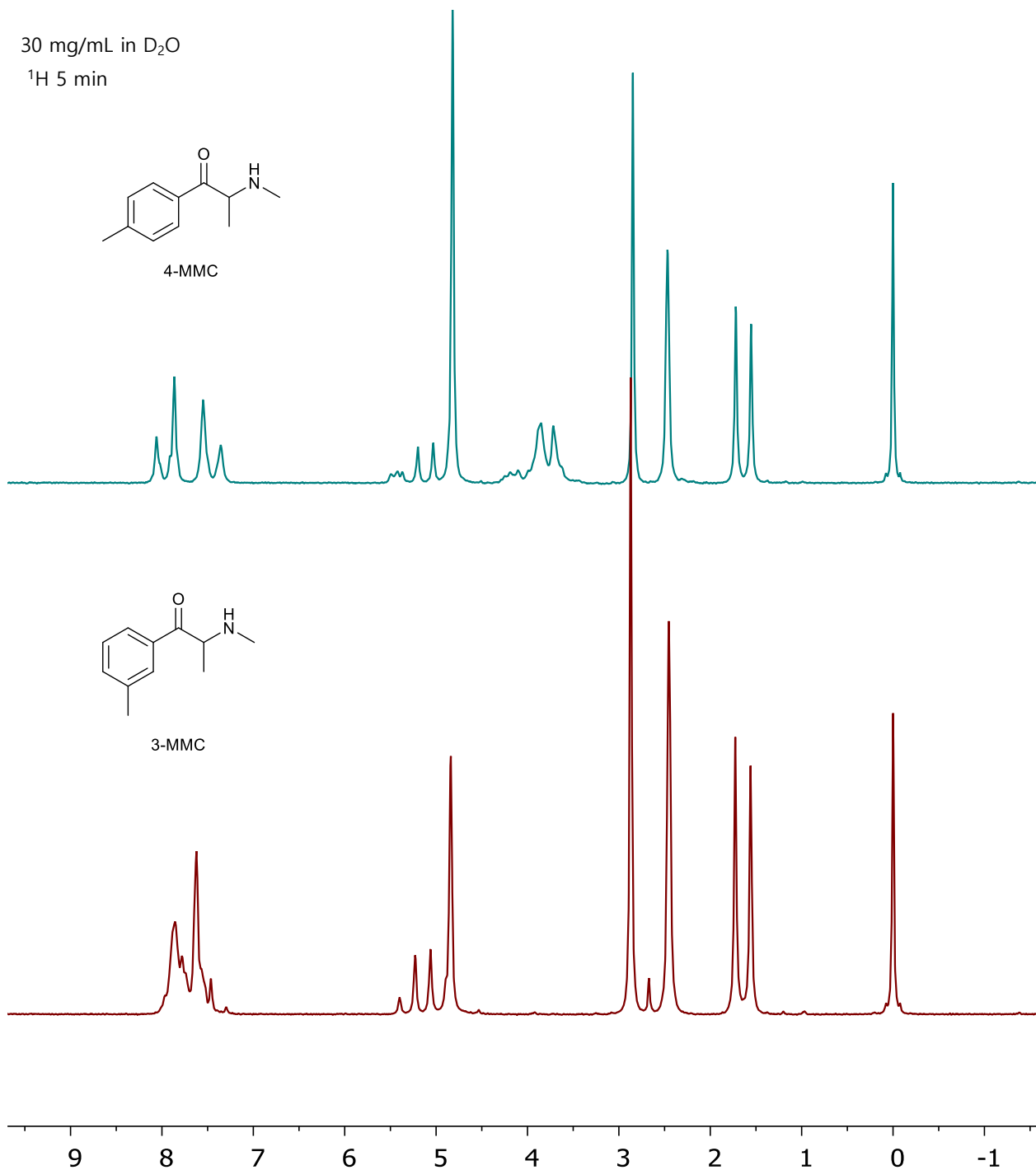
← 6-MAM
 ← AC
 ← Heroin

Street heroin sample
 30 mg/mL in CDCl₃
 1H 5 min

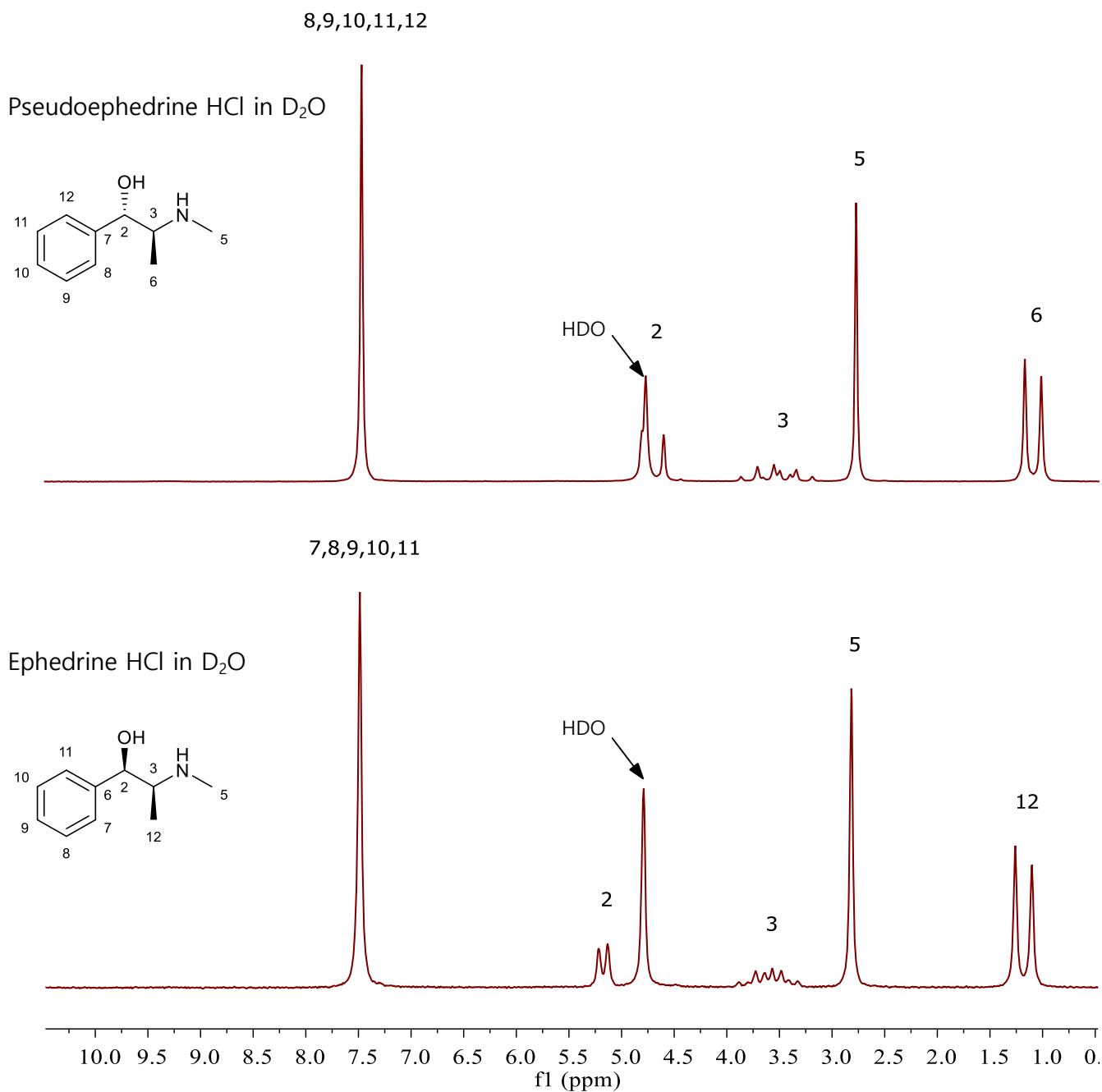


Isomers

In most cases, GC-MS and IR struggle to distinguish isomers. NMR can easily identify these methylmethcathinone (MMC) isomers found in real street samples.

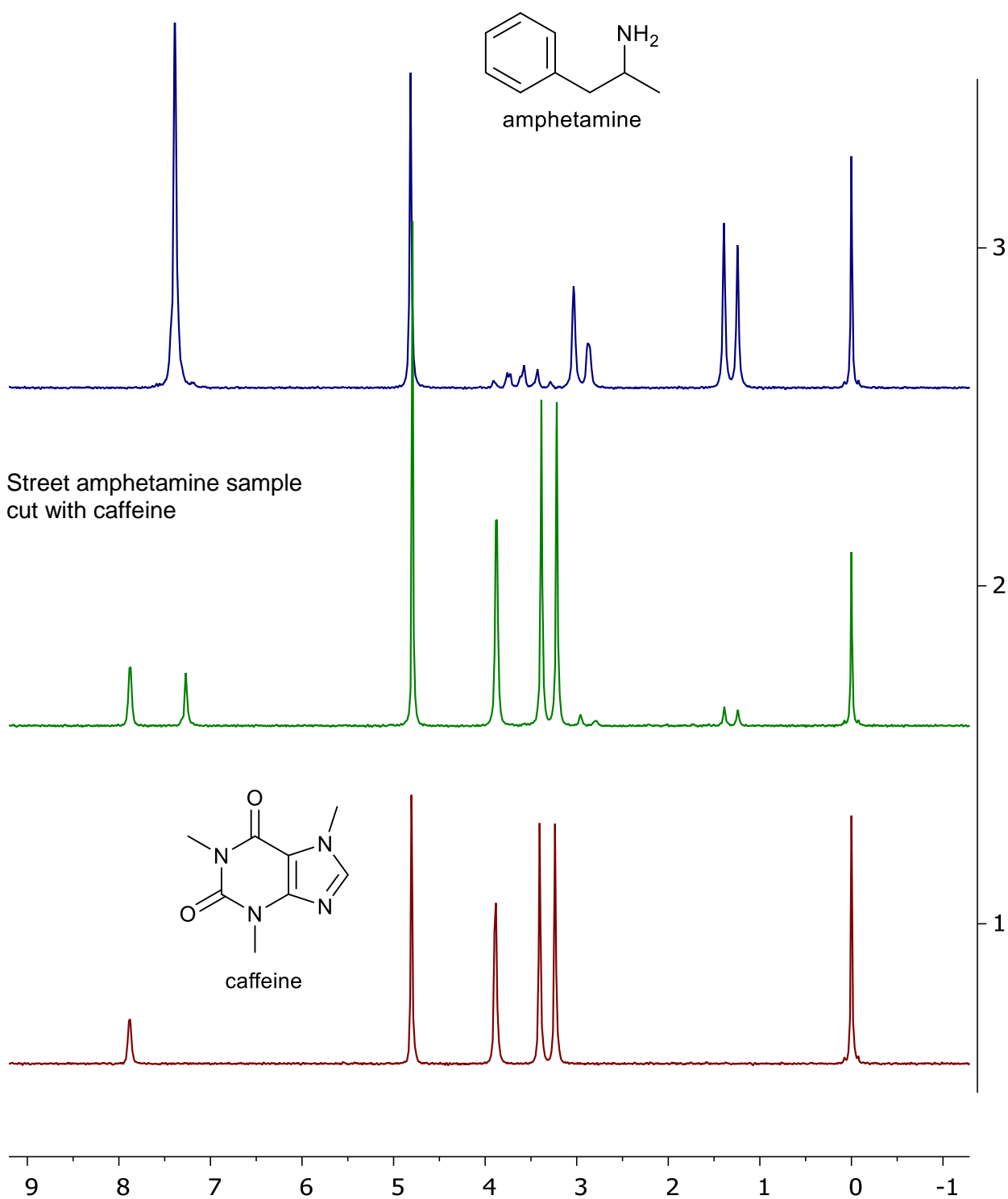


Similarly, ephedrine and pseudoephedrine can be distinguished from each other.



Cutting agents

Many street samples also include cutting agents. Below is an example of amphetamine cut with caffeine, and the two certified reference standards for comparison.



Base or Hydrochloride Salt

Many drug compounds exist as the base or hydrochloride salt, which have different properties and are therefore used differently. For example, the hydrochloride salt of cocaine is a powder that is usually taken intranasally whereas the base has a lower melting point and can be smoked. The two forms can be distinguished using NMR.

