FORENSIC

Narcotics-Profiler

Application note

Innovation with Integrity

Fighting widespread substances of abuse is a constant battle for global law enforcement. Cross-border trafficking continues to be dominated by two major types of compounds: classical narcotics and New Psychoactive Substances (NPS), where seize and control are of increasing importance.

The United Nations Office on Drugs and Crime (UNODC) reported 1,124 different compounds found in 135 countries by January 24, 2022. Each substance in both groups (narcotics and NPS) can occur in their pure form, or within a mixture of other scheduled and non-scheduled substances. Jurisdiction requires identification and quantification of any scheduled substance for legal proceedings, whereas comprehensive profiling of all constituents present in seized material adds value to the criminal investigators for clustering cases (Figure 1).
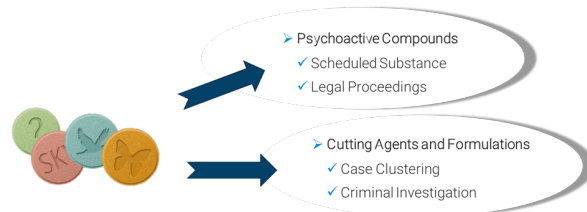
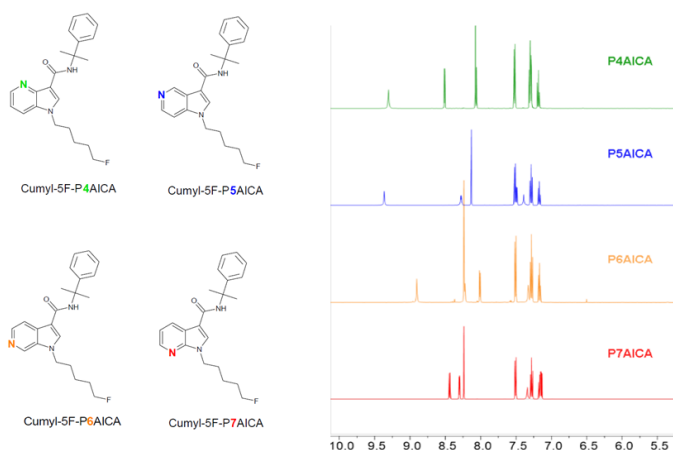**Figure 1** The task: disclosure of substances present in a mixture

Forensic Analysis by NMR

The application of Nuclear Magnetic Resonance (NMR) is widely accepted worldwide to analyze suspicious material on a molecular level. Its capability to deliver targeted and untargeted identification and quantification of known and unknown substances is the most prominent advantage of this key technology (Figure 2). By means of NMR, known molecular structures are verified and new molecular structures are elucidated. Additionally, the quantification of substances, even in a mixture, is also achieved by NMR without the need for compound specific reference material. The only limitations up to now for this technology to be deployed even more widely have been the need for spectroscopic expert knowledge and certain infrastructure and investment requirements for these highly sophisticated, floor-standing analytical instruments.

Figure 2 The power of NMR in narcotics analysis
Source: Bachelorthesis, J. Riedel, HS Fresenius, Germany, 2019

The Bruker Fourier 80 benchtop NMR system now extends the deployment capabilities of NMR significantly (Figure 3).

Through the use of its conventional floor standing NMR equipment, Bruker already supports many clients working in police, customs, federal, state, and border control laboratories in over 40 countries across the world. The expertise gained through these partnerships has been used to create custom forensic analysis solutions. New standards have been established in terms of non-expert usage, method harmonization, expertise exchange, and training synergies.

New end-to-end push-button solution

Bruker now introduces the first comprehensive end-to-end solution for forensic analysis: The Fourier 80 CrimeLab with NMR Narcotics Profiling module. This solution is based on the high-performance 80 MHz benchtop NMR system Fourier 80, including a higher throughput automated sample changer of up to 120 samples. The instrument is operated by the industry-standard TopSpin™ NMR software. The GoScan™ graphical user interface provides a straightforward push button operator experience. Whilst having set new standards already, this state-of-the-art instrument is now bundled with a novel software-based workflow from sample to report, featuring total profiling of compounds present in seized materials. This new concept eliminates the need for spectral data interpretation, making it applicable to any forensic laboratory. The open database approach provides forensic investigators with unrivaled capabilities in tailoring the solution to regional requirements and, therefore, quickly adapting to new threats.

The Fourier 80 CrimeLab with NMR Narcotics Profiling module comes with an initial spectral database of 87 purified scheduled and non-scheduled substances. This database can be easily expanded by adding new entries by following a precise standard operating procedure, by sharing databases across forensic networks, and by non-commercial law enforcement forensic data sharing platforms such as the NPS-Datahub operated by the Drug Enforcement Administration (DEA) of the United States of America and the Federal Criminal Police Office of Germany (BKA).
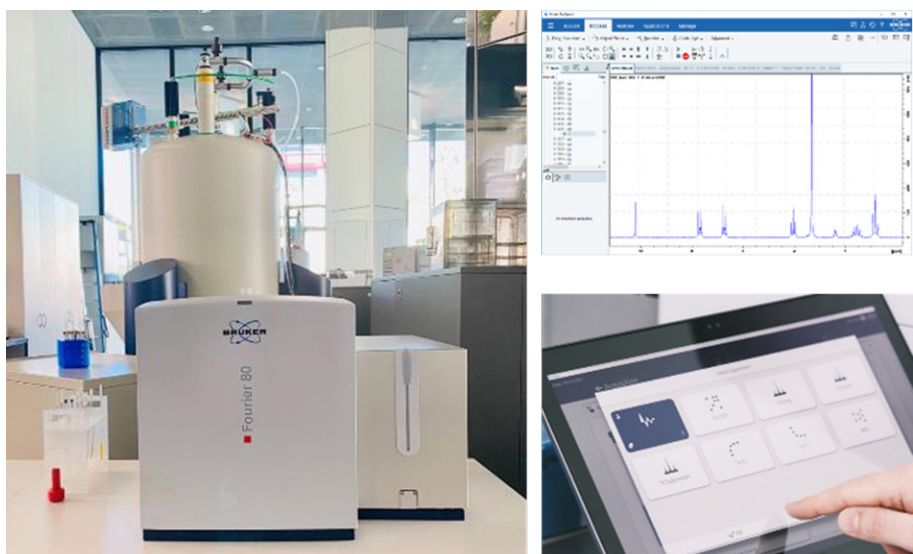

Figure 3 Unique to Bruker: floor-standing and benchtop NMR with same operating software
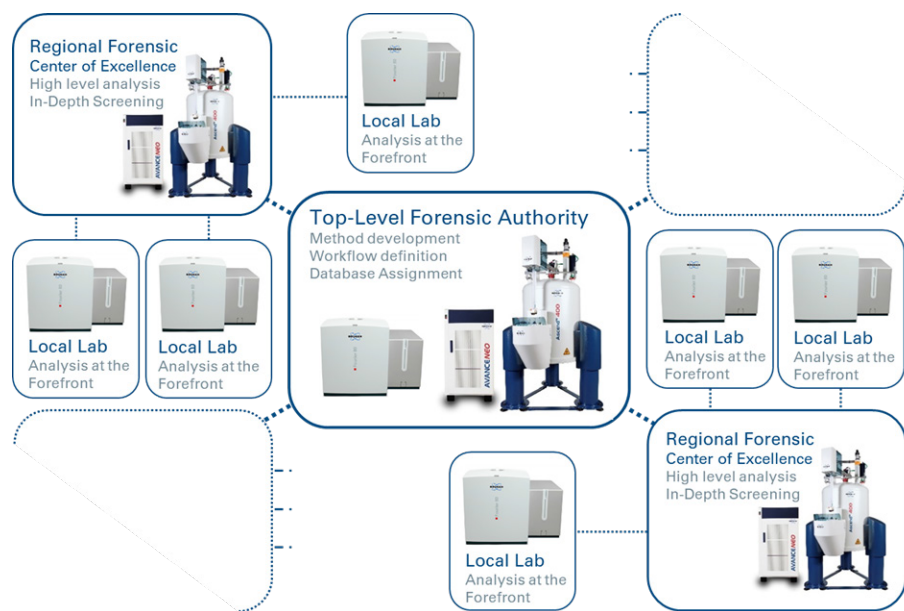

Figure 4 Distributed Laboratory Topology

The analytical results are presented in a Portable Document Format (PDF) and in an interactive NMR spectrum visualization software. Reports include an easy-to-read table (Figure 5) with substances identified and quantified, graphical feedback on substances matched to database entries (Figure 6), and a residual plot for analysis consistency measurement (Figure 7). The reports have been designed to be suitable for legal proceedings.

Signals in the NMR spectrum, that cannot be matched to an existing database entry will be highlighted in the report, calling for further investigation. This could be scheduled or non-scheduled substances, triggering escalation within the Distributed Laboratory Topology (DLT) concept (Figure 4).

Forensic authorities around the world have commissioned over 100 floor-standing Bruker Avance Series NMR systems that use the very same TopSpin NMR software. NMR experts at these forensic centres of excellence could remotely connect with the Fourier 80 system, utilizing the well known and familiar operating software. If this first step of analysis fails to identify the nature of the unknown substance, the ambiguous samples can be sent directly in the NMR sample tube to the closest collaborating forensic laboratory for more detailed analysis. After successful identification of the new substance, it can then be added to the Fourier 80 CrimeLab Narcotics Profiler database by following the described extension principles. Going forward, the new substance will be identified and quantified in non-expert mode again: the solution adapted to a new NPS threat.
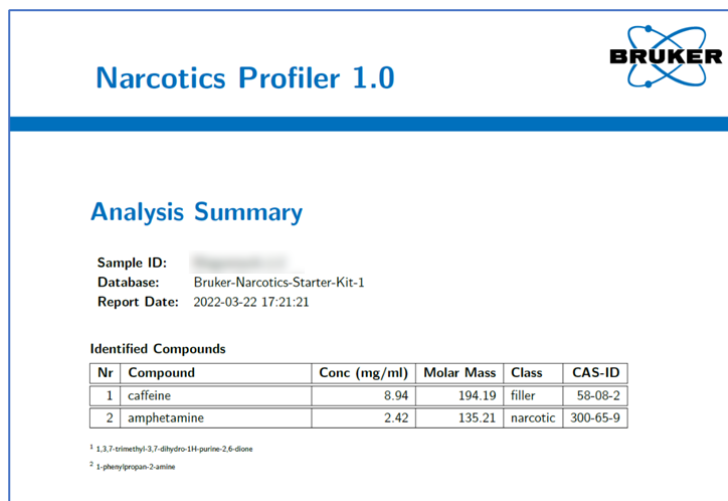

Figure 6 Left side: color-coded database entries to re-build the current NMR spectrum (black). Right side: Residual plot (red) of current spectrum (black) and matched database entries. The significant pattern in the red line indicates that there is a substance present in the sample which cannot be assigned to a database entry.
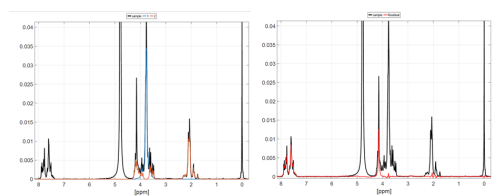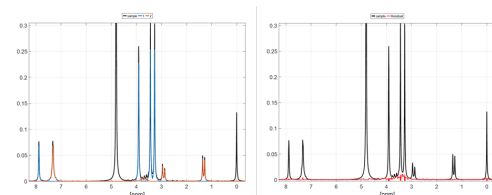

Figure 7 Left side: color-coded database entries to re-build the current NMR spectrum (black). Right side: Residual plot (red) of current spectrum (black) and matched database entries. The flat red line indicates that all signals and so all substances in the mixture have been successfully identified.

Conclusion

Bruker's unique Distributed Laboratory Topology concept for forensic networks features floor-standing and benchtop NMR systems, including smart deployment strategies. The unparalleled analytical power of NMR can now be applied in narcotics forensics more broadly, acknowledging various infrastructure requirements and operator experience levels. Routine analysis of suspicious substances can be carried out within a push-button workflow, significantly reducing time-to-result. The transparent report, in combination with an open database approach, enables law enforcement to quickly adapt to changing situations.

Narcotics Profiler 1.0

Analysis Summary

Sample ID:
Database: Bruker-Narcotics-Starter-Kit-1
Report Date: 2022-03-22 17:21:21

Identified Compounds

Nr	Compound	Conc (mg/ml)	Molar Mass	Class	CAS-ID
1	caffeine	8.94	194.19	filler	58-08-2
2	amphetamine	2.42	135.21	narcotic	300-65-9

[1] 1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione
[2] 1-phenylpropan-2-amine

Figure 5 Report page 1

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Customer Support
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Online information
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