



## K61 Method Optimization for the Derivatization of 35 Drugs Commonly Reported in Driving Under the Influence of Drugs (DUID) Cases

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**Learning Overview:** After attending this presentation, attendees will have an increased understanding of which derivatizing agent and technique are best suited for the analysis of a variety of common drugs of differing chemistries.

**Impact on the Forensic Science Community:** This presentation will impact the forensic science community by providing forensic laboratories with a derivatization and Gas Chromatography/Mass Spectrometry (GC/MS) method for Tier 1 drugs and metabolites associated with DUID cases.

DUID encompasses prescription, over-the-counter, and controlled substances that cause impairment of one's judgment and motor skills. A series of recommendations has been published that describes two tiers of drugs that are commonly seen in DUID cases.<sup>1</sup> Screening and confirmatory cutoff limits have been recommended for the Tier 1 drugs to create better consistency across laboratories.<sup>1</sup>

Typical casework for many forensic toxicology laboratories for DUIDs includes blood and urine screenings. There is a move internationally from GC to Liquid Chromatography (LC) techniques, but many laboratories still lack instrumentation such as a triple quadrupole LC/MS/MS. For most laboratories, derivatization is therefore a critical step for certain drugs to be suitable for GC/MS analysis.

The Tier 1 drugs consist of four classes of drugs. The Central Nervous System (CNS) stimulants include methamphetamine, amphetamine, 3,4-methylenedioxymethamphetamine (MDMA), 3, 4-methylenedioxyamphetamine (MDA), cocaine, benzoylecgonine, and cocaethylene. The CNS depressants consist of carisoprodol, meprobamate, zolpidem, alprazolam,  $\alpha$ -hydroxyalprazolam, clonazepam, 7-aminoclonazepam, lorazepam, diazepam, nordiazepam, oxazepam, and temazepam. Codeine, 6-acetylmorphine, buprenorphine, norbuprenorphine, fentanyl, hydrocodone, hydromorphone, methadone, morphine, oxycodone, oxymorphone, tramadol, and o-desmethyltramadol make up the narcotic analgesic category. The cannabis category includes Tetrahydrocannabinol (THC), carboxy-THC, and 11-hydroxy-THC. Differences in the functional groups associated with these drugs often require different derivatizing reagents such as silylation, acylation, and alkylation reagents. This research aims to determine a single GC/MS method for the analysis of all 35 recommended Tier 1 drugs and metabolites.

A test mix was prepared by adding 1mL of a 10 $\mu$ g/mL solution for each of the 35 drugs in acetonitrile. Seven derivatizing reagents, Pentafluoropropionic Acid Anhydride (PFPA), Trifluoroacetic Acid Anhydride (TFAA), Heptafluorobutyric Anhydride (HFAA), N, O-Bis (Trimethylsilyl)Trifluoroacetamide with 1% Trimethylchlorosilane (BSTFA with 1% TMCS), N-Methyl-N-Trimethylsilylfluoroacetamide (MSTFA), N-methyl-N-(tert-butyltrimethylsilyl) trifluoroacetamide with 1% Tert-Butyltrimethylchlorosilane (MTBSTFA with 1% TBDMCS), and Trimethylanilinium Hydroxide (TMAH) were assessed. Triplicate samples of 100  $\mu$ L of the test mix were derivatized for each reagent changing the temperature and time of incubation followed by GC/MS analysis.

Separation of all 35 drugs was achieved on an Agilent® 6890 GC 5975 MS using an Agilent® DB-5MS Ultra Inert (30m x 0.25mm x 25 $\mu$ m) capillary column with a temperature program starting at 60°C and ending at 325°C. MSTFA and PFPA yielded the most consistent results across the range of chemistries of the drugs and it was possible to obtain sharp, reproducible baseline-resolved peaks at concentrations equal to the cutoff values stated in the DUID recommendations for the 35 Tier 1 drugs and metabolites.<sup>1</sup>

### Reference(s):

1. Barry K. Logan, Amanda L. D'Orazio, Amanda L.A. Mohr, Jennifer F. Limoges, Amy K. Miles, Colleen E. Scarneo, Sarah Kerrigan, Laura J. Liddicoat, Karen S. Scott, Marilyn A. Huestis. Recommendations for Toxicological Investigation of Drug-Impaired Driving and Motor Vehicle Fatalities—2017 Update. *Journal of Analytical Toxicology*, Volume 42, Issue 2, 1 March 2018, Pages 63–68, <https://doi-org.arcadia.idm.oclc.org/10.1093/jat/bkx082>.

### Derivatization, GC/MS Analysis, DUID