

Novel Psychoactive Substances

Certified Reference Materials for
Forensic Analysis, Clinical Toxicology
& Drug Testing

Reference Materials
for accurate results

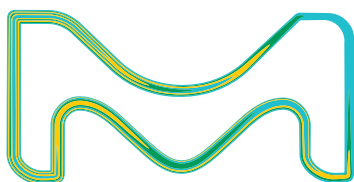


Table of contents

Reference Materials for Novel Psychoactive Substances

Amphetamines	4
Analgesics (non-opioid)	6
Benzodiazepines.....	7
Benzyl & Phenyl Piperazines	9
Synthetic Cannabinoids	10
Cathinones	12
Cocaine analogues.....	14
Fentanyls	15
Hallucinogens	17
Opiates & Opioids	18
Phenethylamines	19
Pipradrols & Piperidines	19



Consistency is Our Standard.

We produce reference materials! Not research chemicals!

Novel Psychoactive Substances (NPS) are newly misused narcotic or psychotropic compounds, comparable to classic psychotropic substances, that may pose a threat to public health. NPS drugs are typically analogs and synthetic derivatives of naturally occurring compounds, existing controlled substances, or research chemicals used during the development of pharmaceuticals, designed to produce effects similar to the controlled substances they mimic. Illicit and legal sources of NPS promote them as “legal highs”, “research chemicals”, and “designer drugs” or as products labeled “not for human consumption”, “plant food” or “bath salts” to circumvent regulations. NPS are diverse and include many drug classes, such as amphetamines, analgesics, benzodiazepines, benzyl & phenyl piperazines, cannabinoids, cathinones, cocaine analogs, fentanyls, hallucinogens, opiates and opioids, phenethylamines, pipradrols and piperidines, and a range of prescribed medications. NPS drugs are currently emerging at an unprecedented rate worldwide.

Our high standards match yours

Our Cerilliant® brand offers the widest selection of high-quality Certified Reference Materials (CRMs) for novel psychoactive substances including parent drugs, metabolites, impurities, and degradants, as well as their stable-labeled internal standards. These certified reference materials are fully characterized under ISO/IEC 17025 and ISO 17034 accreditation; their solutions are gravimetrically prepared using precision

balances that have been qualified to ensure minimal uncertainty, flame sealed under argon into ampoules for long term shelf life and are rigorously tested through accelerated and real time studies to ensure accuracy and shelf life. These solution-based CRMs are suitable for numerous applications from forensic analysis, clinical toxicology, urine drug testing, or pharmaceutical research to pain management and prescription monitoring. They can be used as calibrators and controls or for quantitation, including isotope dilution methods by GC/MS or LC/MS. Since many NPS are classified as controlled substances, Cerilliant® solution-based certified reference materials are offered in a convenient, DEA-exempt format designed to improve laboratory efficiency.

Cerilliant® certified solution standards and Certified Spiking Solutions® are manufactured and tested to the highest industry standards including ISO 17034, ISO/IEC 17025, ISO 13485 and ISO 9001. Each certified reference material is supported by a comprehensive Certificate of Analysis which provides all analytical data on stability, homogeneity, accuracy of concentration as compared to an independently prepared multi-point calibration curve, and uncertainty and traceability information to support regulatory requirements.

Cerilliant® CRM are designed to promote laboratory efficiency, ensure accuracy and reliability of results and support laboratory regulatory requirements. We provide accurate reference materials, saving you from doubt and uncontrolled uncertainty caused by the use of research grade chemicals for with calibration.

We know only the most accurate and reliable analytical product will do.

That's why we offer the Supelco® portfolio of reference materials, including our Cerilliant® ready-to-use solution standards. Whatever your needs, our portfolio is always fit for purpose, ensuring your results are accurate, precise and reproducible, and your systems fully certified.

Our comprehensive portfolio, developed by analytical chemists for analytical chemists, covers a broad range of analytical solutions, and every product is meticulously quality-controlled to maintain the integrity of your testing protocols.

And with Supelco® scientists dedicated to your analytical applications, the expertise you need is always on hand.

Amphetamines

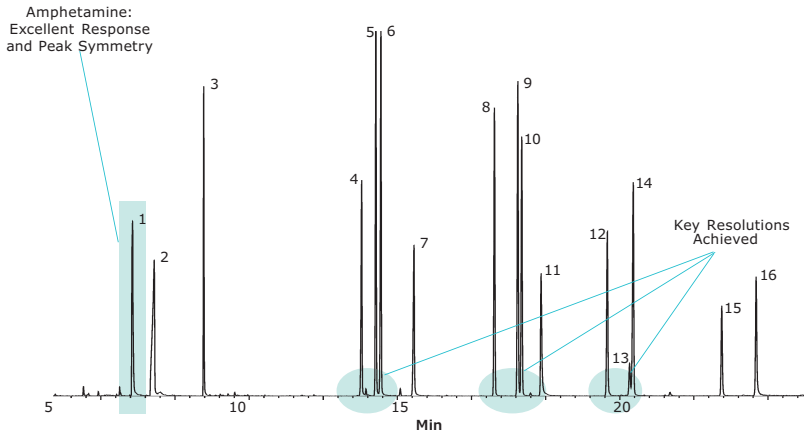
Amphetamines have an extended history of abuse seen throughout the world. This drug class includes amphetamine and its derivatives, which are predominantly central nervous system stimulants responsible for increasing alertness and focus, improving mood, decreasing fatigue, and reducing appetite. Many amphetamines are legally used to treat attention deficit hyperactivity disorder (ADHD), narcolepsy and depression or are prescribed as weight-loss drugs. Amphetamines can also produce euphoria and psychedelic effects and are therefore sold as “designer drugs” on the illicit drug market. Amphetamines have a high potential for abuse and psychological addiction.



Cat. No.	Product Description
Amphetamines	
A-007-1ML	(±)-Amphetamine, 1.0 mg/mL in methanol
A-013-1ML	(±)-Amphetamine-D ₅ (deuterium label on side chain), 1.0 mg/mL in methanol
M-013-1ML	(±)-MDMA, 1.0 mg/mL in methanol
M-029-1ML	(±)-MDMA-D ₅ , 1.0 mg/mL in methanol
M-009-1ML	(±)-Methamphetamine, 1.0 mg/mL in methanol
M-060-1ML	(±)-Methamphetamine-D ₁₁ , 1.0 mg/mL in methanol
H-136-1ML	4-Hydroxyamphetamine HCl, 1.0 mg/mL (as free base) in methanol
H-133-1ML	4-Hydroxyamphetamine-D ₅ HBr, 100 µg/mL (as free base) in methanol
F-056-1ML	Fenproporex HCl, 1 mg/mL (as free base) in methanol
F-057-1ML	Fenproporex-D ₅ HCl, 100 µg/mL in methanol
P-127-1ML	Phendimetrazine tartrate, 1.0 mg/mL in methanol
P-132-1ML	Phendimetrazine-D ₅ HCl, 100 mg/mL (as free base) in methanol
P-128-1ML	Phenmetrazine HCl, 1mg/mL in methanol
P-129-1ML	Phenmetrazine-D ₅ HCl, 100 µg/mL (as free base) in methanol

 New

GC Analysis of Basic Drugs using an Equity®-5 Column

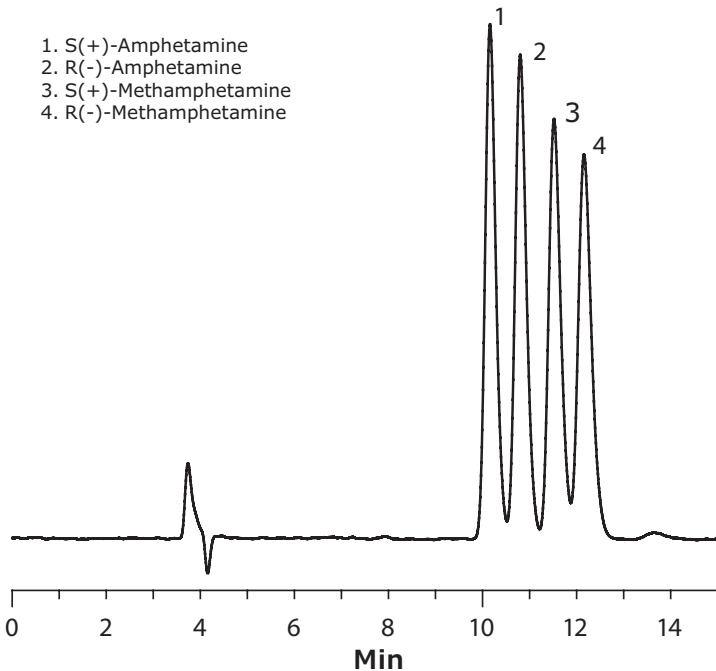


- | | |
|--------------------|-----------------|
| 1. Amphetamine | 10. Cocaine |
| 2. Methamphetamine | 11. Desipramine |
| 3. Nicotine | 12. Codeine |
| 4. Caffeine | 13. Morphine |
| 5. Diphenhydramine | 14. Diazepam |
| 6. Lidocaine | 15. Heroin |
| 7. Phenobarbital | 16. Fentanyl |
| 8. Methadone | |
| 9. Amitriptyline | |

Conditions

column	Equity®-5, 30 m x 0.25 mm I.D., 0.25 µm (28089-U)
oven	45 °C (2 min), 25 °C/min to 110 °C, 15 °C/min to 200 °C, 6 C/min to 280 °C (3 min)
carrier gas	helium, 40 psi for 0.2 min then 0.7 mL/min constant flow
sample	~15 ng on-column of a 16-component drug standard
injection	0.3 µL pulsed splitless @ 50 mL/min (0.5 min)
liner	2 mm I.D., splitless
inj. temp.	250 °C
MSD interface	325 °C
scan range	m/z = 40-450

HPLC Analysis of Amphetamine and Methamphetamine Enantiomers on Astec® CHIROBIOTIC® V2 column



1. S(+)-Amphetamine
2. R(-)-Amphetamine
3. S(+)-Methamphetamine
4. R(-)-Methamphetamine

Resolution of the enantiomers of methamphetamine and amphetamine is of clinical interest for two reasons: they exhibit different physiological effects, and it is a means to distinguish between legal and illicit sources of the drugs. Shown here is the rapid and efficient resolution of all four enantiomers on an Astec® CHIROBIOTIC® V2 column

Conditions

column	Astec® CHIROBIOTIC® V2, 25 cm x 4.6 mm I.D., 5 µm (15024AST)
column temp.	40 °C
mobile phase	[A] methanol; [B] water; [C] acetic acid; [D] ammonium hydroxide; (95:5:0.1:0.02, A:B:C:D)
flow rate	1 mL/min
pressure	840 psi (58 bar)
sample	100 µg/mL each enantiomer in methanol
injection	5 µL
detector	UV, 205 nm

To read more visit us at SigmaAldrich.com/amphetamines-chiral-HPLC

Analgesics (non-opioid)

Non-opioid analgesics include non-steroidal anti-inflammatory drugs (NSAIDs), selective COX-2 inhibitors, and acetaminophen. NSAIDs have potent anti-inflammatory, analgesic and antipyretic activity, and are particularly effective in the management of musculoskeletal pain.



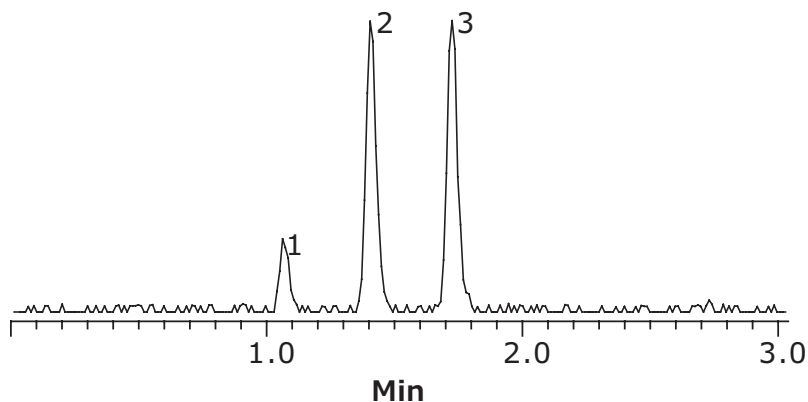
Cat. No.	Product Description
Analgesics (non-opioid)	
M-007-1ML	(±)-Methadone, 1.0 mg/mL in methanol
M-021-1ML	(±)-Methadone-D ₃ , 1.0 mg/mL in methanol
M-089-1ML	(±)-Methadone-D ₅ , 1.0 mg/mL in methanol
A-064-1ML	Acetaminophen, 1.0 mg/mL in methanol
P-917-1ML	Acetaminophen-D ₄ , 1.0 mg/mL in methanol
P-909-1ML	Acetaminophen-D ₄ , 100 µg/mL in methanol
A-113-1ML	AH-7921 HCl 1.0 mg/mL (as free base) in methanol
A-114-1ML	AH-7921-D ₃ HCl, 100 µg/mL (as free base) in methanol
T-027-1ML	cis-Tramadol HCl, 1.0 mg/mL (as free base) in methanol
D-167-1ML	N-Desmethyl U-47700, 1.0 mg/mL in acetonitrile
D-168-1ML	N-Desmethyl U-47700-D ₃ , 100 µg/mL in acetonitrile
D-023-1ML	N-Desmethyl-cis-tramadol HCl, 1.0 mg/mL (as free base) in methanol

Cat. No.	Product Description
D-110-1ML	N-Desmethyl-cis-tramadol-D ₃ HCl, 100 µg/mL (as free base) in methanol
N-089-1ML	Normeperidine, 1.0 mg/mL in methanol
N-083-1ML	Normeperidine-D ₄ , 1.0 mg/mL in methanol
D-058-1ML	O-Desmethyl-cis-tramadol-D ₆ , 100 µg/mL (as free base) in methanol
T-058-1ML	Tapentadol HCl, 1.0 mg/mL (as free base) in methanol
T-059-1ML	Tapentadol-D ₃ HCl, 100 µg/mL (as free base) in methanol
T-067-1ML	Tapentadol-D ₃ -β-D-glucuronide, 100 µg/mL in 1:1 acetonitrile:water
T-060-1ML	Tapentadol-β-D-glucuronide, 100 µg/mL in 1:1 acetonitrile:water
T-020-1ML	Tramadol-13C ₃ D ₃ HCl, 1.0 mg/mL (as free base) in methanol
W-004-1ML	W-18, 1 mg/mL in acetonitrile

New

LC-MS Analysis of Methadone and Metabolites EDDP and EMDP on Ascentis® Express RP Amide

1. EDDP (2-Ethylidene-1,5-dimethyl-3,3-diphenylpyrrolidine)
2. Methadone
3. EMDP (2-Ethyl-5-methyl-3,3-diphenylpyrrolidine)



Conditions

column	Ascentis® Express RP Amide, 10 cm x 2.1 mm I.D., 2.7 µm particles (53913-U)
column temp.	35 °C
mobile phase	[A] 10 mM ammonium formate in water, pH 3.6; [B] 10 mM ammonium formate in acetonitrile, pH 3.6; (65:35, A:B)
flow rate	0.5 mL/min
sample	200 µg/L in 25:75, water:acetonitrile
injection	0.5 µL
detector	ESI(+), m/z 100-1000

Benzodiazepines

Benzodiazepines, sometimes called “benzos”, possess sedative, hypnotic, anxiolytic, anticonvulsant, muscle relaxant, and amnesic actions, which are useful for treating a variety of indications such as alcohol dependence, seizures, anxiety disorders, panic, agitation, and insomnia.

Benzodiazepines have been available for over 50 years, but recently, their use has increased significantly. Over-prescription has resulted in large populations of long-term users becoming physically dependent on benzodiazepines and has also led to leakage of synthetic analogs into the illicit drug market. Like opioids, benzodiazepines have a depressant effect on the central nervous system and therefore can cause respiratory depression at high doses. They are frequently found in combination with opioid analgesics in postmortem toxicology, but they are rarely identified as the only drug involved.

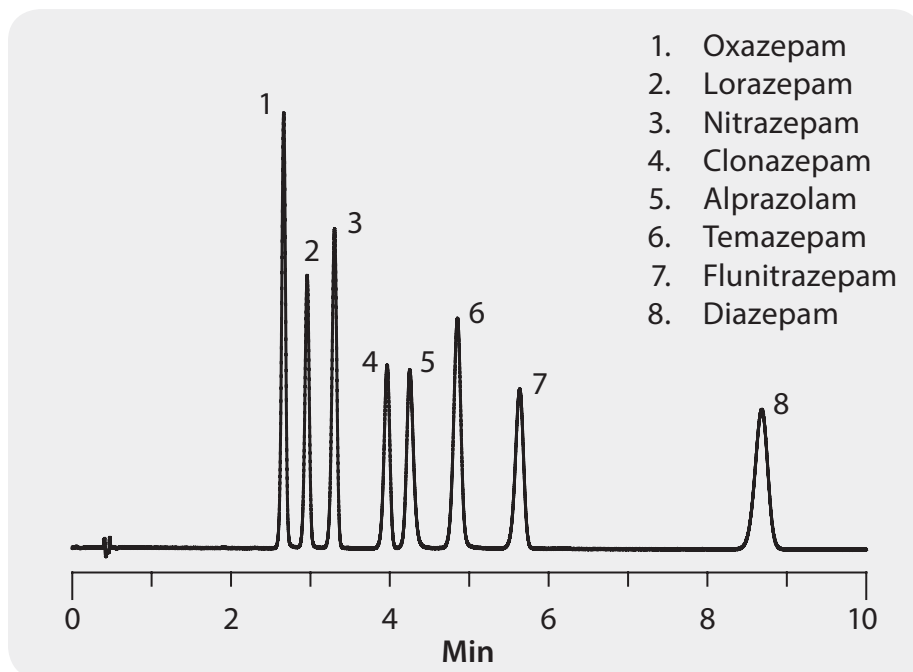


Cat. No.	Product Description
Benzodiazepines	
A-903-1ML	Alprazolam, 1.0 mg/mL in methanol
A-902-1ML	Alprazolam-D ₅ , 100 µg/mL in methanol
C-176-1ML	Camazepam, 1 mg/mL in acetonitrile
C-167-1ML	Clonazolam, 1 mg/mL in acetonitrile
C-168-1ML	Clonazolam-D ₄ , 100 µg/mL in acetonitrile
D-163-1ML	Delorazepam-D ₄ , 100 µg/mL in acetonitrile
D-156-1ML	Deschloroetizolam, 1 mg/mL in methanol
D-159-1ML	Diclazepam, 1 mg/mL in acetonitrile
D-160-1ML	Diclazepam-D ₄ , 100 µg/mL in acetonitrile
F-047-1ML	Flubromazolam, 1.0 mg/mL in methanol
F-003-1ML	Flurazepam, 1.0 mg/mL in methanol
F-044-1ML	Flurazepam-D ₄ , 100 µg/mL in methanol
L-049-1ML	Loprazolam, 1 mg/mL in 90:10 Acetonitrile:DMSO (v/v)
M-197-1ML	Meclonazepam, 1 mg/mL in methanol
M-198-1ML	Meclonazepam-D ₃ , 100 µg/mL in methanol
M-205-1ML	Medazepam, 1 mg/mL in methanol
N-117-1ML	Nifoxipam, 1 mg/mL in 90:10 acetonitrile:DMSO (v/v)
N-118-1ML	Nifoxipam-D ₄ , 100 µg/mL in 90:10 acetonitrile:DMSO (v/v)
N-125-1ML	Nortetrazepam, 1 mg/mL (as free base) in methano
Q-006-1ML	Quazepam, 1 mg/mL in acetonitrile
T-124-1ML	Tetrazepam, 1 mg/mL in acetonitrile
Z-020-1ML	Zolazepam HCl, 1 mg/mL (as free base) in methanol
H-129-1ML	α-Hydroxyetizolam, 100 µg/mL in methanol

For a complete product listing visit us at SigmaAldrich.com/cerilliant

 New

RP-HPLC Analysis of Benzodiazepines using an Ascentis® Express Biphenyl

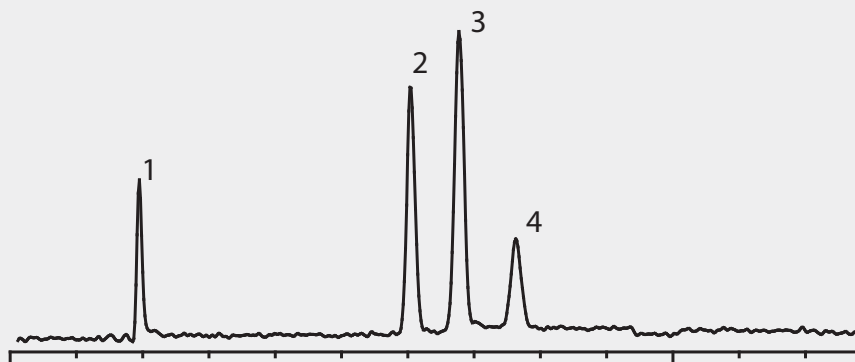


Conditions

column	Ascentis® Express Biphenyl, 10 cm x 3.0 mm I.D., 2.7 µm particles (64066-U)
column temp.	35 °C
mobile phase	[A] Water; [B] acetonitrile; (70:30, A:B)
flow rate	1.0 mL/min
pressure	5294 psi (365 bar)
sample	Benzodiazepine multicomponent Mixture-8 (B-033-1mL) diluted to 50µg/mL in 50:50 Water:Methanol
injection	1.0 µL
detector	UV, 254 nm

LC/MS Analysis of Benzodiazepines using an Ascentis® Phenyl Column

1. Fenoldopam (10 µg/mL) (M+H)⁺ = 306.08
2. Lorazepam (10 µg/mL) (M+H)⁺ = 321.01
3. Notrazepam (10 µg/mL) (M+H)⁺ = 282.08
4. Clonazepam (10 µg/mL) (M+H)⁺ = 316.04



Benzyl & Phenyl Piperazines

Piperazine derivatives are abused as illicit drugs worldwide. The phenylpiperazines 3-chlorophenylpiperazine (mCPP) and Trifluoromethylphenylpiperazine (TFMPP) have less desirable psychotropic effects compared with MDMA, a related stimulant. Benzyl piperazine (BZP) is an indirect dopamine and noradrenaline agonist without serotonergic properties and has stimulant effects in humans. The clinical toxicity of BZP mainly includes hallucinations, agitation, seizures, and hyperthermia. Illicit drug manufacturers are selling mCPP, TFMPP and BZP as an alternative to “Ecstasy”; therefore, piperazines are commonly found in ecstasy pills as substitutes for MDMA. Public health risks and the high abuse potential of these products have led to their legal control in several regions, such as the US, Europe, and Australia.



Cat. No.	Product Description
Benzyl & Phenyl Piperazines	
C-089-1ML	1-(3-Chlorophenyl)piperazine (mCPP) HCl, 1.0 mg/mL (as free base) in methanol
C-112-1ML	1-(3-Chlorophenyl)piperazine-D ₈ HCl, 100 µg/mL (as free base) in methanol
T-045-1ML	3-Trifluoromethylphenylpiperazine (TFMPP) HCl, 1.0 mg/mL (as free base) in methanol
T-920-1ML	3-Trifluoromethylphenylpiperazine-D ₄ (TFMPP) HCl, 100 µg/mL (as free base) in methanol
B-906-1ML	Benzyl piperazine diHCl, 1.0 mg/mL (as free base) in methanol
B-907-1ML	Benzyl piperazine-D ₇ diHCl, 100 µg/mL (as free base) in methanol

 New

For a comprehensive portfolio of reference materials & CRMs visit us at SigmaAldrich.com/standards

More details on our Forensic Testing Workflow Solutions can be found at SigmaAldrich.com/forensic

Synthetic Cannabinoids

Synthetic cannabinoids mimic the effects of THC and are sold in herbal incense or smoking blend packets, known by a number of brand names including K2, Spice, Black Mamba, Bombay Blue, Genie, Zohai, Banana Cream Nuke, Krypton, Lava Red, and many more. The introduction of synthetic cannabinoids, originally designed to aid in academic research of multiple sclerosis, AIDS and chemotherapy, have greatly increased cannabis selection and ready access on the internet or from local head shops and gas stations. They are often called “synthetic marijuana”, “natural herbs”, “herbal incense”, or “herbal smoking blends” and are frequently labeled “not for human consumption”. Lately, synthetic cannabinoids are increasingly offered in e-cigarette form as “c-liquid” with brand names such as Kronic. Within the last few years, synthetic cannabinoids have grown to be one of the most widely abused drug classes worldwide.

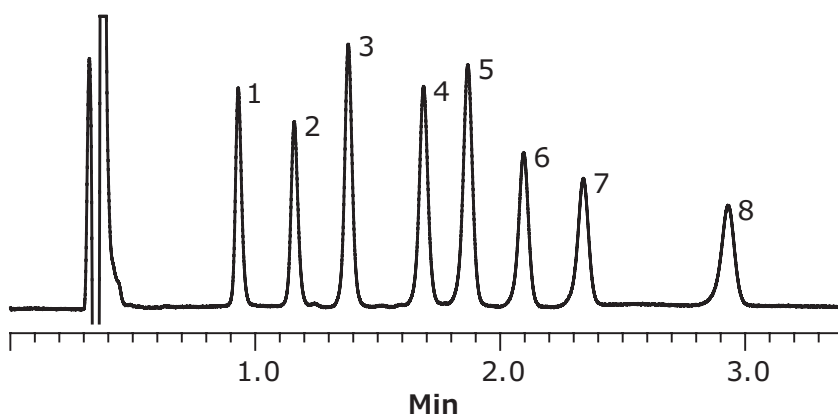


Cat. No.	Product Description
Synthetic Cannabinoids	
S-101-1ML	5-Fluoro PB-22 3-carboxyindole metabolite, 100 µg/mL in acetonitrile
S-107-1ML	AB-CHMINACA metabolite M4, 100 µg/mL in acetonitrile
S-108-1ML	AB-CHMINACA, 100 µg/mL in methanol
S-103-1ML	BB-22 3-carboxyindole metabolite, 100 µg/mL in acetonitrile
S-104-1ML	BB-22, 100 µg/mL in acetonitrile
S-112-1ML	FUB-APINACA, 100 µg/mL in methanol
S-025-1ML	JWH-018 (Spice Cannabinoid), 100 µg/mL in methanol
S-035-1ML	JWH-018 4-Hydroxypentyl metabolite, 100 µg/mL in methanol
S-039-1ML	JWH-018 4-Hydroxypentyl metabolite-D ₅ (indole-D ₅), 100 µg/mL in methanol
S-054-1ML	JWH-018 5-Hydroxypentyl metabolite, 100 µg/mL in methanol
S-033-1ML	JWH-018 5-Pentanoic acid metabolite, 100 µg/mL in methanol
S-109-1ML	MAB-CHMINACA, 100 µg/mL in methanol
S-105-1ML	MAM2201 5-Pentanoic acid metabolite, 100 µg/mL in methanol
S-118-1ML	MMB-CHMICA, 100 µg/mL in methanol
S-111-1ML	MMB-FUBINACA, 100 µg/mL in acetonitrile
S-102-1ML	PB-22 3-carboxyindole metabolite, 100 µg/mL in acetonitrile
S-094-1ML	PB-22 4-Hydroxypentyl metabolite, 100 µg/mL in acetonitrile
S-095-1ML	PB-22 4-Hydroxypentyl metabolite-D ₅ (indole-D ₅), 100 µg/mL in acetonitrile
S-096-1ML	PB-22 5-Pentanoic acid metabolite, 100 µg/mL in acetonitrile
S-097-1ML	PB-22 5-Pentanoic acid metabolite-D ₅ (indole-D ₅), 100 µg/mL in acetonitrile
S-076-1ML	PB-22, 100 µg/mL in acetonitrile
S-119-1ML	SDB-005, 100 µg/mL in acetonitrile
S-077-1ML	UR-144 5-Hydroxypentyl metabolite, 100 µg/mL in methanol
S-079-1ML	UR-144 5-Hydroxypentyl metabolite-D ₅ (indole-D ₅), 100 µg/mL in methanol
S-078-1ML	UR-144 5-Pentanoic acid metabolite, 100 µg/mL in methanol

 New

HPLC Analysis of Spice Cannabinoids on an Ascentis® Express F5 column

- | | |
|----------------------------|-------------------|
| 1. JWH-073 metabolite | 5. HU-210, HU-211 |
| 2. JWH-200 | 6. JWH-250 |
| 3. CP-47, 497 | 7. JWH-073 |
| 4. CP-47, 497 C8 homologue | 8. JWH-018 |



Conditions

column	Ascentis® Express F5, 10 cm x 2.1 mm I.D., 2.7 µm particles (53569-U)
column temp.	30 °C
mobile phase	[A] 50 mM ammonium formate; [B] water; [C] acetonitrile; (10:35:55, A:B:C)
flow rate	0.6 mL/min
pressure	4075 psi (281 bar)
sample	100 µg/mL in 45:55 water:acetonitrile
injection	3 µL
detector	UV, 200 nm

For our offering on cannabis testing please visit us at
[SigmaAldrich.com/cannabis](https://www.sigmaaldrich.com/cannabis)

Cathinones

Cathinone-based stimulants emerged as a regulatory and societal threat in the Europe, Asia, and US in late 2010.

Marketed as “bath salts”, “psychoactive bath salts” or “PABS” in head shops and on the internet, these synthetic cathinones offer recreational highs that mimic the effects of illegal drugs such as cocaine, methamphetamine, and LSD. Bath salt products, sometimes also called “plant food”, “jewelry cleaner” or “phone screen cleaner,” are sold in powder or crystalline form under names including Bliss, Cloud Nine, Lunar Wave, Vanilla Sky and White Lightning. Packaging labels list the compounds as “not for human consumption”, a tactic used to circumvent regulatory control and maintain legal status. According to Drug Enforcement Administrations worldwide, bath salt cathinones have grown increasingly popular due to their ready availability over the internet and their still often perceived “legal status”.

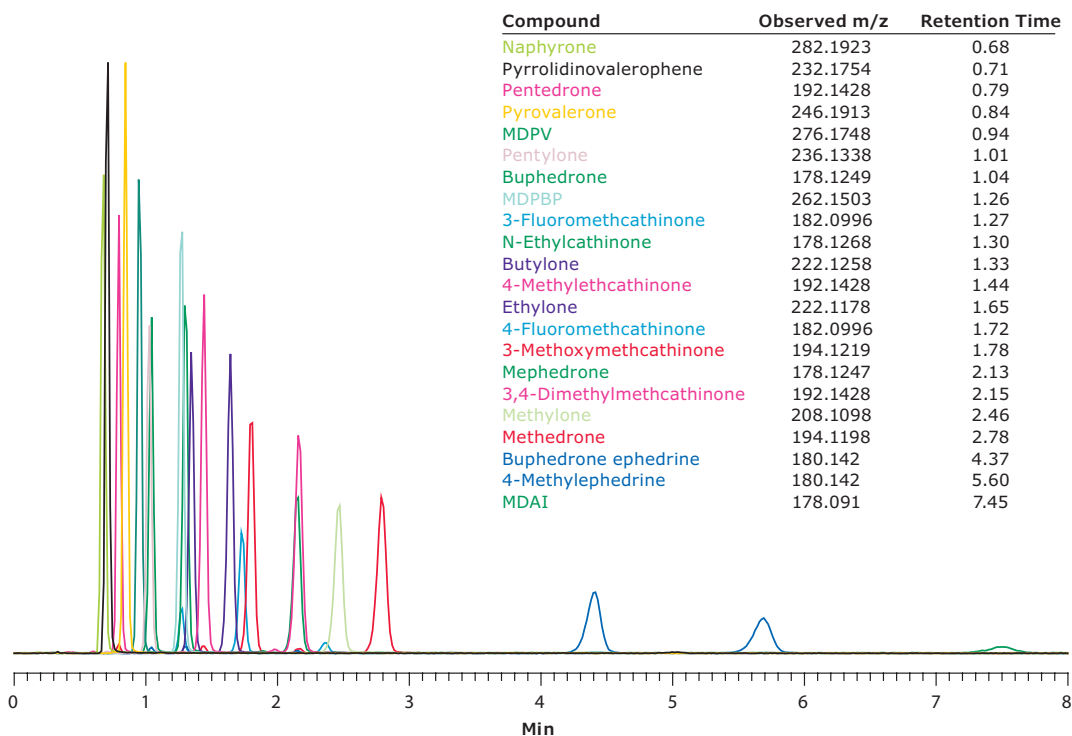


Cat. No.	Product Description
Cathinones	
B-072-1ML	4-Bromomethcathinone HCl (4-BMC HCl), 1 mg/mL (as free base) in methanol
C-169-1ML	4-Chloroethcathinone HCl, 1 mg/mL (as a free base) in methanol
C-170-1ML	4-Chloroethcathinone-D ₅ HCl, 100 µg/mL as free base in methanol
C-174-1ML	4-Chloromethcathinone HCl (4-CMC HCl), 1 mg/mL (as free base) in methanol
C-173-1ML	4-Cl-α-PPP HCl, 1 mg/mL (as free base) in methanol
C-172-1ML	4-Cl-α-PVP HCl, 1 mg/mL (as free base) in methanol
M-199-1ML	4-Methyl-N-ethyl-pentedrone HCl (4-MEAP HCl)
D-161-1ML	Dibutylone HCl, 1.0 mg/mL (as free base) in methanol
D-162-1ML	Dibutylone-D ₃ HCl, 100 µg/mL (as free base) in methanol
E-071-1ML	Ethylone HCl, 1.0 mg/mL (as free base) in methanol
E-072-1ML	Ethylone-D ₅ HCl, 100 µg/mL (as free base) in methanol
E-129-1ML	N-Ethylpentylone HCl, 1 mg/mL (as free base) in methanol
E-130-1ML	N-Ethylpentylone-D ₅ HCl, 100 µg/mL (as free base) in methanol
T-121-1ML	TH-PVP HCl, 1 mg/mL (as free base) in methanol
P-100-1ML	α-Pyrrolidinopropiophenone HCl (α-PPP HCl), 1.0 mg/mL (as free base) in methanol
P-090-1ML	α-Pyrrolidinovalerophenone HCl (α-PVP HCl), 1.0 mg/mL (as free base) in methanol
P-101-1ML	α-Pyrrolidinovalerophenone D ₈ HCl (α-PVP D ₈ HCl), 100 µg/mL (as free base) in methanol

 New

Fast LC-MS Analysis of Twenty-Two Illicit Phenethylamine and Cathinone “Bath Salts”, including Isobarics, or Isobaric compounds in Saliva on an Ascentis® Express HILIC column after Extraction using SPME LC Tips

This application enabled the resolution of the five groups of isobaric compounds under ideal MS conditions. Other coelutions are not a problem because they are not isobaric and will be distinguished in the mass spectrometer. Regarding sample prep, this experiment employed for the extraction of analytes biocompatible SPME LC fibers, which are suitable for clinical, bioanalytical or forensic applications requiring extraction of compounds of interest from a variety of biological matrices prior to LC/MS analysis. With the spiked saliva samples, SPME LC gave five- to ten-fold increase in detected analytes compared to the traditional “dilute and shoot” method. For spiked plasma samples, compared to standard protein precipitation, the SPME LC technique showed ten-fold reduction in detected matrix and over two-fold increase in response for the analytes tested



Conditions

sample/matrix	Human saliva adjusted to pH 3.0 with formic acid and spiked at 20 ng/mL with the twenty-two Bath Salts compounds. A 200 µL aliquot of saliva was placed into a 300 µL conical 96-well collection plate.
SPME fiber SPME LC Tip	extraction SPME LC fibers were preconditioned in 50:50 methanol:water and placed into sample wells. Extraction was performed for 15 minutes on an IKA VORTEX MS3 shaker at 500 rpm. desorption Fibers were then desorbed in 100 µL of 0.5% ammonium hydroxide in methanol for 60 minutes at 500 rpm vortex. (Desorbed samples were then evaporated and reconstituted in 40 µL of acetonitrile and analyzed directly.)
column	Ascentis® Express HILIC, 5 cm x 2.1 mm I.D., 2.7 µm (53934-U)
mobile phase	5 mM ammonium formate (98:2 acetonitrile:water)
flow rate	0.6 mL/min
pressure	1262 psi (87 bar)
column temp.	35 °C
detector	ESI(+), 100-1000 m/z
injection	1.0 µL

Cocaine Analogues

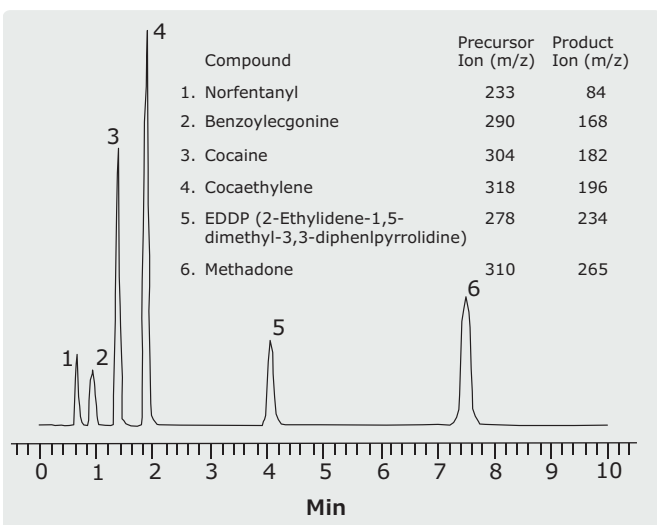
Cocaine is a strong addictive illicit stimulant with appetite suppressant and topical anesthetic properties. The free-base form of cocaine, known as “crack”, can be smoked by users for a quicker high. Cocaine is globally one of the most frequently used illegal drugs with the highest consumption rates detected in North America followed by Europe and South America. Cocaine is addictive and after continued use, there is high risk that dependence will occur. Cocaine sold on the illicit market is often mixed with local anesthetics, cornstarch, quinine, or sugar, which can result in additional toxicity.



Cat. No.	Product Description
Benzoyllecognine	
B-001-1ML	Benzoyllecgonine-D ₃ , 100 µg/mL in methanol
B-004-1ML	Benzoyllecgonine, 1.0 mg/mL in methanol
Cocaine	
C-004-1ML	Cocaine-D ₃ , 100 µg/mL in acetonitrile
C-008-1ML	Cocaine, 1.0 mg/mL in acetonitrile
H-119-1ML	m-Hydroxycocaine, 1.0 mg/mL in acetonitrile
H-121-1ML	o-Hydroxycocaine, 1.0 mg/mL in acetonitrile
H-135-1ML	p-Hydroxycocaine HCl, 1.0 mg/mL (as free base) in acetonitrile
N-003-1ML	Norcocaine HCl, 1.0 mg/mL (as free base) in acetonitrile
N-034-1ML	Norcocaine-D ₃ HCl, 100 µg/mL (as free base) in acetonitrile
Ecognine	
E-001-1ML	Ecgonine methyl ester, 1.0 mg/mL in acetonitrile
E-002-1ML	Ecgonine methyl ester-D ₃ , 100 µg/mL in acetonitrile
E-004-1ML	Ecgonine HCl, 1.0 mg/mL (as free base) in methanol

New

LC/MS Analysis of Illicit Drugs as Standards on Ascentis® Express RP-Amide



Conditions

column: Ascentis® Express RP-Amide, 10 cm x 2.1 mm I.D., 2.7 µm (Product No. 53913-U)
 mobile phase: 10 mM ammonium formate in water:acetonitrile (75:25);
 flow rate: 0.2 mL/min
 column temp: 35 °C
 detector: ESI+, MRM (see table for transitions)
 injection: 2 µL
 sample: illicit drug standards, each 200 ng/mL in mobile phase;
 instrument: Agilent 1100 with ABI-3200 QTRAP

Fentanyl

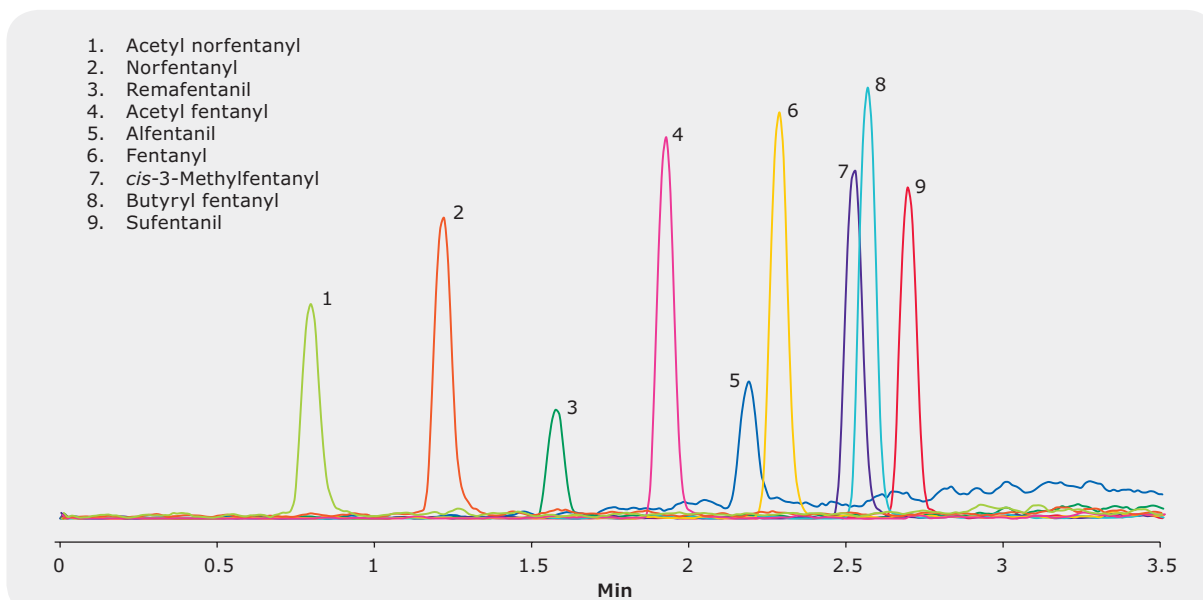
The emergence of fentanyl as a drug of abuse represents the greatest challenge to current forensic toxicology. Recently, a huge number of new fentanyl structural variants, also known as designer fentanyls, have appeared on the illicit drug market. Often mixed with traditional opioid drugs, these highly potent fentanyl analogues have caused harmful intoxications and dramatically increased opioid related mortality in the United States, Europe and Asia. Due to the very high potency of some fentanyl analogues, forensic testing labs are facing the challenge of detecting minimal trace amounts of drug in biological samples while ensuring laboratory safety.



Cat. No.	Product Description
Fentanyls	
H-130-0.5ML	(±)-β-Hydroxythiofentanyl HCl, 100 µg/mL (as free base) in methanol
A-139-0.5ML	4-ANPP, 100 µg/mL in methanol
A-157-0.5ML	4-ANPP-D ₅ , 100 µg/mL in methanol
F-050-0.5ML	4-Fluoroisobutyrylfentanyl, 100 µg/mL in methanol
A-140-0.5ML	Acryl fentanyl HCl, 100 µg/mL (as free base) in methanol
C-162-1EA	Carfentanil oxalate, 100 µg/mL in methanol
C-163-1EA	Carfentanil-D ₅ oxalate, 100 µg/mL (as free base) in methanol
C-177-0.5ML	Cyclopropyl fentanyl HCl, 100 µg/mL (as free base) in methanol
F-013-1ML	Fentanyl, 1.0 mg/mL in methanol
F-001-1ML	Fentanyl-D ₅ , 100 µg/mL in methanol
F-046-0.5ML	Furanyl fentanyl HCl, 100 µg/mL (as free base) in methanol
F-053-0.5ML	Furanyl fentanyl-D ₅ HCl, 100 µg/mL (as free base) in methanol
I-038-0.5ML	Isobutyryl fentanyl HCl, 100 µg/mL (as free base) in methanol
M-200-0.5ML	Methoxyacetyl fentanyl HCl, 100 µg/mL (as free base) in methanol
N-114-1EA	Norcarfentanil oxalate, 100 µg/mL (as free base) in methanol
O-047-0.5ML	Ocfentanil, 100 µg/mL in methanol
F-054-0.5ML	ortho-Fluorofentanyl HCl, 100 µg/mL (as free base) in methanol
F-048-0.5ML	para-Fluorobutyryl fentanyl (PFBF), 100 µg/mL in methanol
F-049-0.5ML	para-Fluorofentanyl, 100 µg/mL in methanol
V-048-0.5ML	Valeryl fentanyl HCl, 100 µg/mL (as free base) in methanol
V-068-0.5ML	Valeryl fentanyl-D ₅ HCl, 100 µg/mL (as free base) in methanol

New

LC-MS/MS Analysis of Fentanyl and Fentanyl Analogs



Conditions

column	Ascentis® Express Biphenyl, 5 cm x 2.1 mm I.D., 2.7 µm particles (64057-U)
column temp.	50 °C (ambient)
mobile phase	[A] 0.1% formic acid in water ; [B] 0.1% formic acid in methanol
gradient	20% B to 40% B in 1 min, then to 50% B in 1 min, then to 80% B in 1 min, then hold 80% B for 1 min, then to 20% in 0.1 min, then hold 20% B for 1.4 min
flow rate	0.6 mL/min
pressure	5076 psi (350 bar)
sample	250 pg/mL in 90:10 methanol:water
injection	1 µL
detector	MS/MS, ESI(+), MRM data requested from Bellefonte (Emily Barrey, Cory Muraco)

For our offer on Clinical Mass Spectrometry Workflows, visit us at

SigmaAldrich.com/clinical

Hallucinogens

From plant-based psychoactive substances, phencyclidine (PCP) derivatives, and tryptamines to lysergic acid diethylamide (LSD), hallucinogens—also known as psychedelics—remain popular drugs of abuse due to their ability to alter perception, thought, emotion, and consciousness. Abuse of hallucinogenic substances is widely prevalent around the world. Over the last few years, synthetic and plant-based hallucinogenic substances have appeared on the clandestine drug market. These emerging hallucinogens produce sedating and anesthetizing effects in addition to distorting the sensory perceptions of users. Newer hallucinogens include Kratom, *Salvia divinorum*, Khat and PCP. Tryptamines, a class of hallucinogens that includes drugs such as 5-methoxy-DMT and 5-methoxy-DALT, represent approximately 10 percent of total new psychoactive compounds.



Cat. No.	Product Description
Dissociatives	
P-007-1ML	PCP (Phencyclidine), 1.0 mg/mL in methanol
P-006-1ML	PCP-D ₅ (Phencyclidine-D ₅), 1.0 mg/mL in methanol
P-003-1ML	PCP-D ₅ (Phencyclidine-D ₅), 100 µg/mL in methanol
LSD	
L-001-1ML	LSD (Lysergic acid diethylamide), 1.0 mg/mL in acetonitrile
L-002-1ML	LSD-D ₃ (Lysergic acid diethylamide-D ₃), 100 µg/mL in acetonitrile
NBOMe Analogs	
B-061-1ML	25B-NBOMe HCl, 1.0 mg/mL (as free base) in methanol
B-062-1ML	25B-NBOMe-D ₃ HCl, 100 µg/mL (as free base) in methanol
C-131-1ML	25C-NBOMe HCl, 1.0 mg/mL (as free base) in methanol
C-132-1ML	25C-NBOMe-D ₃ HCl, 100 µg/mL (as free base) in methanol
Plant-based	
S-098-1ML	(-)-Scopolamine HBr, 1.0 mg/mL (as free base) in 10% water in acetonitrile
S-099-1ML	(-)-Scopolamine-D ₃ HCl, 100 µg/mL (as free base) in 10% water in acetonitrile
H-099-1ML	7-Hydroxymitragynine, 100 µg/mL in 0.1N ammonia in methanol
H-109-1ML	7-Hydroxymitragynine-D ₃ , 100 µg/mL in 0.1N ammonia in methanol
M-152-1ML	Mitragynine, 100 µg/mL in methanol
M-182-1ML	Mitragynine-D ₃ , 100 µg/mL in methanol
Tryptamines	
M-169-1ML	5-MeO-AMT, 1.0 mg/mL in methanol
M-165-1ML	5-MeO-DALT, 1.0 mg/mL in acetonitrile
M-167-1ML	5-MeO-DiPT, 1.0 mg/mL in methanol
M-168-1ML	5-MeO-DMT, 1.0 mg/mL in methanol
D-102-1ML	N,N-Dimethyltryptamine (DMT), 1.0 mg/mL in methanol

 New

Opiates & Opioids

The drug class of opiates includes psychoactive alkaloid compounds derived from the opium poppy plant *Papaver somniferum*, including morphine, codeine and thebaine. Opioids comprise all natural and synthetic substances that bind to opioid receptors in the brain to produce typical opioid-like effects. Medically, opioids are primarily used for pain relief, anesthesia, suppression of diarrhea or cough and replacement therapy for opioid use disorder. Opioids are frequently misused for their euphoric and psychoactive effects with a high potential of addiction and physical dependence. Acute withdrawal symptoms include severe dysphoria, irritability, sweating, nausea, rhinorrhea, tremor, vomiting and myalgia. All opioids have depressant effects on respiration and have been associated with some overdose deaths and emergency department visits.



Cat. No.	Product Description
buprenorphine	
B-035-1ML	Buprenorphine glucuronide, 100 µg/mL in methanol
B-044-1ML	Buprenorphine, 1.0 mg/mL in methanol
B-060-1ML	Buprenorphine-D ₄ -3-β-D-glucuronide, 100 µg/mL in methanol
B-908-1ML	Buprenorphine-D ₄ , 1.0 mg/mL in methanol
codeine	
H-003-1ML	Hydrocodone, 1.0 mg/mL in methanol
H-008-1ML	Hydrocodone-D ₃ , 1.0 mg/mL in methanol
H-048-1ML	Hydrocodone-D ₆ , 1.0 mg/mL in methanol
N-053-1ML	Norhydrocodone HCl, 1.0 mg/mL (as free base) in methanol
N-054-1ML	Norhydrocodone-D ₃ HCl, 100 µg/mL (as free base) in methanol
morphine	
A-006-1ML	6-Acetylmorphine-D ₃ , 100 µg/mL in acetonitrile
A-009-1ML	6-Acetylmorphine, 1.0 mg/mL in Acetonitrile
M-005-1ML	Morphine, 1.0 mg/mL in methanol
M-006-1ML	Morphine-D ₃ , 1.0 mg/mL in methanol
M-017-1ML	Morphine-3-β-D-glucuronide-D ₃ , 100 µg/mL in methanol with 0.05% NaOH
M-018-1ML	Morphine-3-β-D-glucuronide, 100 µg/mL in methanol:water (1:1)
M-046-1ML	Morphine-6-β-D-glucuronide, 1.0 mg/mL in water:methanol (80:20)
M-120-1ML	Morphine-6-β-D-glucuronide-D ₃ , 100 µg/mL in methanol:water (1:1)

Cat. No.	Product Description
naloxone	
N-004-1ML	Naloxone, 1.0 mg/mL in methanol
N-099-1ML	Naloxone-3β-D-glucuronide, 1.0 mg/mL in 10% water in methanol
N-109-1ML	Naloxone-D ₅ -3-β-D-glucuronide, 100 µg/mL in 10% water in methanol
N-115-1ML	Naloxone-D ₅ , 1.0 mg/mL in methanol
oxycodone	
O-002-1ML	Oxycodone, 1.0 mg/mL in methanol
O-004-1ML	Oxymorphone, 1.0 mg/mL in methanol
O-006-1ML	Oxycodone-D ₃ , 1.0 mg/mL in methanol
O-008-1ML	Oxycodone-D ₆ , 1.0 mg/mL in methanol
O-019-1ML	Oxymorphone-D ₃ , 1.0 mg/mL in methanol
O-030-1ML	Oxymorphone-3-β-D-glucuronide, 100 µg/mL in methanol:water (1:1)
O-031-1ML	Oxymorphone-D ₃ -3-β-D-glucuronide, 100 µg/mL in methanol:water (1:1)
U drugs	
D-167-1ML	N-Desmethyl U-47700, 1.0 mg/mL in acetonitrile
D-168-1ML	N-Desmethyl U-47700-D ₃ , 100 ug/mL in acetonitrile
U-003-1ML	U-47700, 1mg/mL in methanol
U-004-1ML	U-47700-D ₃ , 100 µg/ml in methanol
U-005-1ML	U-51754 HCl, 1 mg/mL (as free base) in methanol
U-006-1ML	U-51754-D ₃ HCl, 100 µg/mL (as free base) in methanol
U-007-1ML	U-50488 mesylate, 1 mg/mL (as free base) in methanol
U-011-1ML	U-48800 HCl, 1 mg/mL (as free base) in methanol

 **New**

Phenethylamines

Phenethylamines represent a class of compounds with documented psychedelic and stimulant effects. The 2C family, which includes structural analogs such as 2C-B and 2C-I, has been well known since the 1970s from the synthetic work of Alexander Shulgin and the influence of his 1991 book "PiHKAL: A Chemical Love Story". Other related phenethylamine groups consist of the ring-substituted D-amphetamines (e.g. DOI, DOB) and the dibenzofurans (e.g. BromoDragonFLY, 2C-B-FLY).



Cat. No.	Product Description
Phenethylamines	
E-083-1ML	2,5-Dimethoxy-4-ethylphenethylamine HCl (2C-E HCl), 1.0 mg/mL (as free base) in methanol
C-122-1ML	2C-B-FLY HCl, 1.0 mg/mL (as free base) in 10% water in acetonitrile
C-133-1ML	2C-B-FLY-D ₄ HCl, 100 µg/mL (as free base) in 10% water in acetonitrile
B-026-1ML	4-Bromo-2,5-dimethoxyphenethylamine HCl (2C-B), 1.0 mg/mL (as free base) in methanol
C-124-1ML	4-Chloro-2,5-Dimethoxyphenethylamine HCl (2C-C HCl), 1.0 mg/mL (as free base) in methanol
I-018-1ML	4-Iodo-2,5-dimethoxyphenethylamine- ¹³ C, ₃ D ₃ HCl (2C-I- ¹³ C, ₃ D ₃ HCl), 100 µg/mL (as free base) in methanol
B-049-1ML	R(-)-Bromo-DragonFLY HCl, 1.0 mg/mL (as free base) in methanol

■ New

Pipradrols & Piperidines

Pipradrols are mild central nervous system stimulants, developed since the 1940s, that are used for treating obesity, narcolepsy, ADHD, depression, schizophrenia and most particularly, for counteracting the symptoms of senile dementia. Most pipradrols are no longer used due to concerns about their abuse potential. Piperidine is listed as a Table II precursor under the United Nations Convention Against Illicit Traffic in Narcotic Drugs and Psychotropic Substances due to its use (peaking in the 1970s) in manufacturing of PCP (1-(1-phenylcyclohexyl)) piperidine and other psychoactive substances.



Cat. No.	Product Description
Dissociatives	
P-007-1ML	PCP (Phencyclidine), 1.0 mg/mL in methanol
P-006-1ML	PCP-D ₅ (Phencyclidine-D ₅), 1.0 mg/mL in methanol
P-003-1ML	PCP-D ₅ (Phencyclidine-D ₅), 100 µg/mL in methanol

■ New



Supelco®

Analytical Products

Merck KGaA
Frankfurter Strasse 250
64293 Darmstadt, Germany

For a comprehensive portfolio of reference materials & CRMs visit us at

[SigmaAldrich.com/standards](https://sigmaaldrich.com/standards)

More details on our Forensic Testing Workflow Solutions can be found at

[SigmaAldrich.com/forensic](https://sigmaaldrich.com/forensic)

For our offer on Clinical Mass Spectrometry Workflows, visit us at

[SigmaAldrich.com/clinical](https://sigmaaldrich.com/clinical)

To Place an order or receive technical assistance:

Customer Service: **[SigmaAldrich.com/customerservice](https://sigmaaldrich.com/customerservice)**

Technical Service: **[SigmaAldrich.com/techservice](https://sigmaaldrich.com/techservice)**

To contact a Standards Specialist: **standardsEU@merckgroup.com**

© 2019 Merck KGaA, Darmstadt, Germany and/or its affiliates. All Rights Reserved. Merck, the vibrant M, Cerilliant and Supelco are trademarks of Merck KGaA, Darmstadt, Germany or its affiliates. All other trademarks are the property of their respective owners. Detailed information on trademarks is available via publicly accessible resources. Photos courtesy of DEA.

Lit. No. MK_BR3505EN Ver. 1.0
2019-20041
08/2019