SWGDRUG and Characterization of New Substances, Library Building and Online Resources for Identification

Scott R. Oulton, SWGDRUG Chair

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History

- You are invited to present in a three person panel on Laboratory Support for Timely Identification of Emerging NPS, to provide
  - A fifteen minute overview of “SWGDRUG and
  - Characterization of New Substances
  - Library Building and
  - Online Resources for Drug Identification” as part of a scientific session. (See full list of sessions below).

THE CENTER FOR FORENSIC SCIENCE RESEARCH & EDUCATION

History

- 1997 DEA & ONDCP co-sponsored TWGDRUG
- 1999 First meeting in Washington, DC
- 1999 SWGDRUG name adopted
- 2001 1st Edition of Recommendations
- 2016 Version 7.1 of Recommendations
- 2017 20th Anniversary
  Annual Meeting (June; St. Louis, MO)

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Mission

To improve the quality of the forensic examination of seized drugs and to respond to the needs of the forensic community by supporting the development of internationally accepted minimum standards, identifying best practices within the international community, and providing resources to help laboratories meet these standards.

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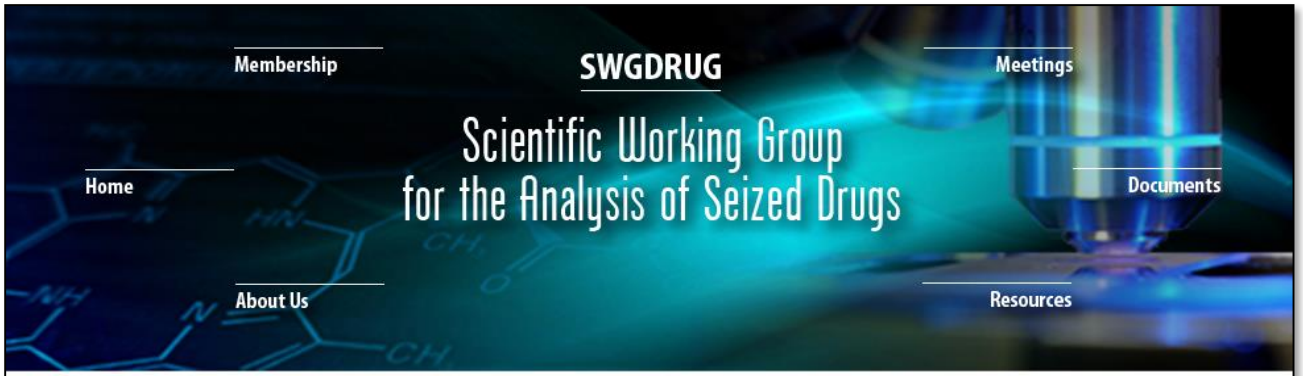
Current Documents

- SWGDRUG Recommendations v. 7.1
- Supplemental Documents:
  - **SD-1:** A Code of Professional Practice for Drug Analysts
  - **SD-2:** Validation of Analytical Methods
  - **SD-3:** Examples of Measurement Uncertainty for Weight Determinations
  - **SD-4:** Examples of Measurement Uncertainty for Purity Determinations
  - **SD-5:** Reporting Examples
  - **SD-6:** Examples of Measurement Uncertainty for Extrapolations of Net Weight and Unit Count
  - **SD-7:** Proposed, Construction of an Analytical Scheme

SWGDRUG Resources



Welcome to the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) Website

What's New:

1) **SWGDRUG Recommendations Version 7.1 was approved on June 9, 2016.**
2) **Supplemental Document (SD-6) was approved on June 9, 2016 and was posted on October 31, 2016. This document provides examples of estimating measurement uncertainty for extrapolations of net weights and unit counts.**
3) **Drug Monographs (being updated regularly), please note the table is now sortable and includes two new columns.**
4) **Searchable Mass Spectral Library Version 3.3 (dated April 16, 2018).**
5) **Searchable Infrared Library Version 1.8 (dated May 31, 2018).**
6) **ENFSI-DWG has published a new Guideline on Sampling of Illicit Drugs for Quantitative Analysis and a corresponding Sampling Calculator, both of which have been posted to this website.**
7) **To keep up with the latest updates (including new monographs, libraries, etc.) from SWGDRUG, follow us on Twitter Follow @swgdrug or email us at swgdrugupdate@gmail.com and ask to be added to our mailing list.**
8) **Check out the first edition of the SWGDRUG Bulletin.**

SWGDRUG Resources

Tools:

The following tools are provided to assist the forensic science community:

- ❑ **SWGDRUG Mass Spectral Library**
- ❑ **SWGDRUG IR Library**
- ❑ **SWGDRUG Drug Monographs**
- ❑ **MS Interpretation Software (NIST MS Interpreter)**
- ❑ **Sampling Probability Calculator for Quantitative Analysis**
  - **ENFSI Validation Report**
  - **ENFSI Sampling Calculator**
- ❑ **Sampling Probability Calculators for Qualitative Analysis**
  - **ENFSI Sampling Calculator Revised July 2017** and **Guidance Document**
  - **CLIC**
- ❑ **Southern Association of Forensic Scientists - Forendex**

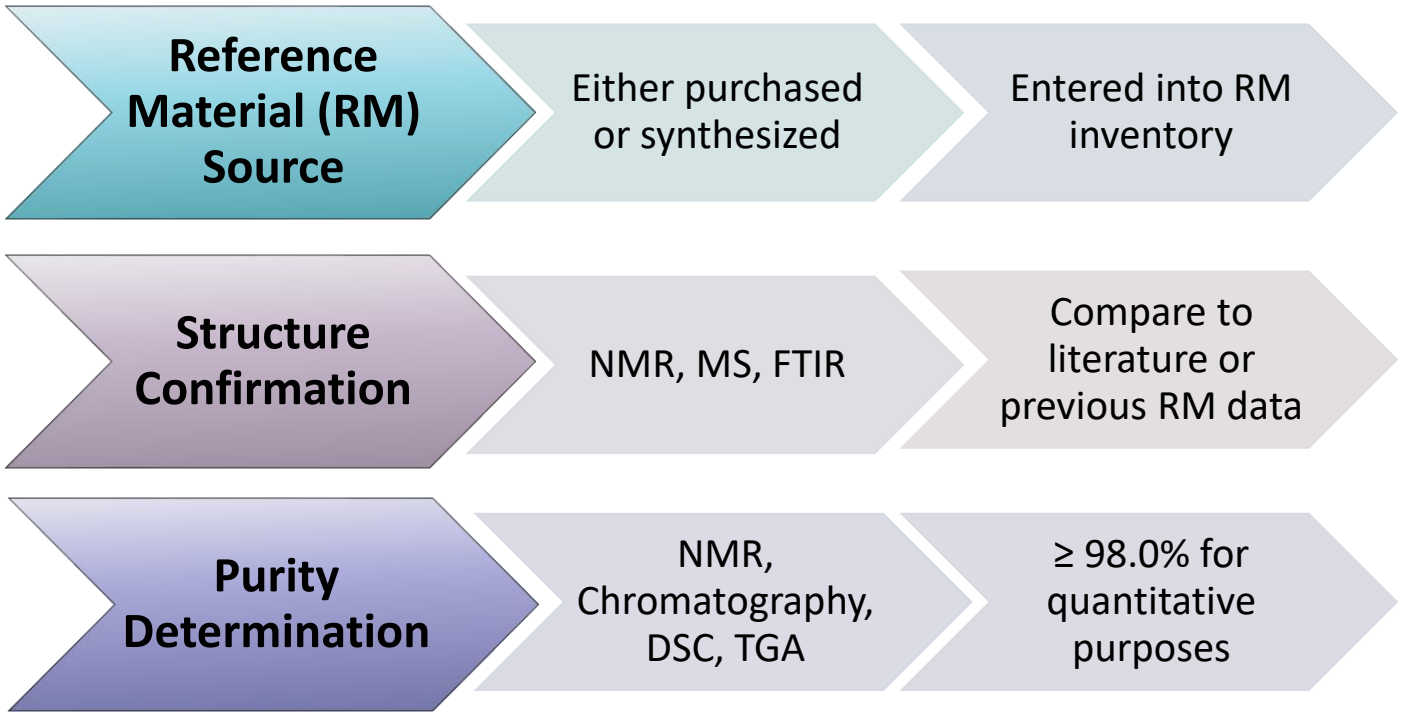
SWGDRUG Resources

- MS Library
  - **Version 3.3c** (September 28, 2018)
  - All spectra collected using EI-MS systems (2850)
  - Several formats (Agilent, Thermo, Shimadzu, etc.)
  - Validated by NIST
- IR Library
  - **Version 1.9** (September 18, 2018)
  - All spectra collected using FTIR-ATR system (> 550)
  - Several formats (Omnic, Opus, PE, etc.)
- Drug Monographs
  - **Approximately 500**

SWGDRUG Monographs

- Produced by DEA Special Testing and Research Laboratory
- Using structurally confirmed RMs
- Intended for the verification of acquired RMs and to provide reviewable analytical data
- Collaborators:
  - Forensic Drug Review
  - The Center for Forensic Science Research and Education

DEA Reference Material Authentication



Process to confirm the identification of a candidate RM or CRM and to determine its purity value and associated uncertainty.

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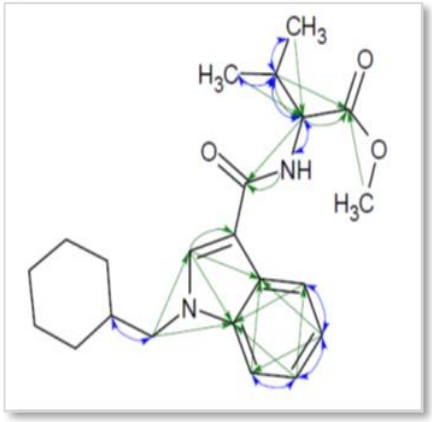
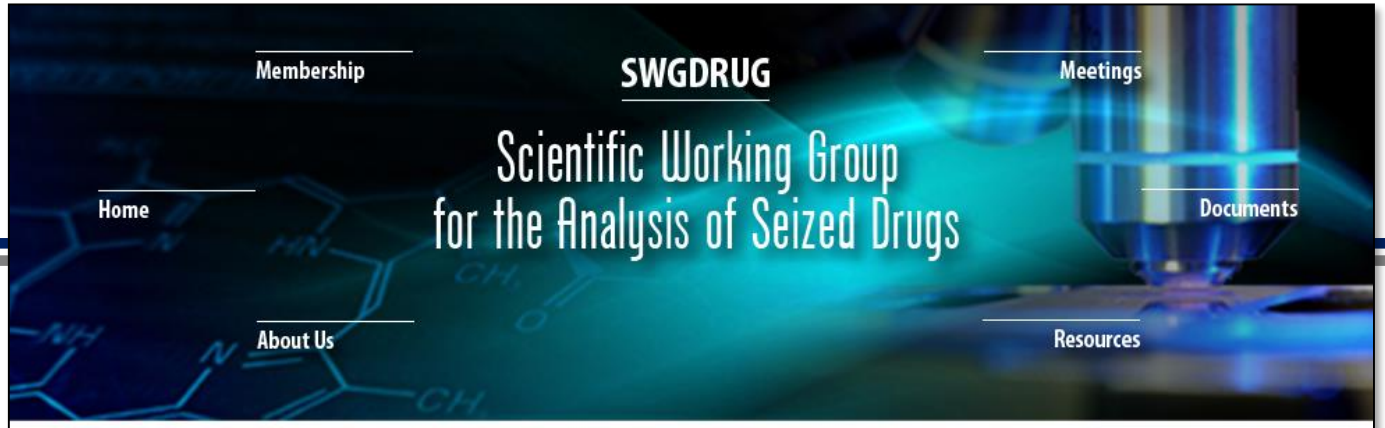
Structural Confirmation

- Verification of structure when no literature or previous lot of a reference material exists for comparison
- NMR Experiments (1D & 2D)
  - Proton NMR (^{1}HNMR)
  - Carbon NMR (^{13}CNMR)
  - Correlation Spectroscopy (COSY)
  - Heteronuclear Single Quantum Coherence (HSQC)
  - Heteronuclear Multiple Bond Correlation (HMBC)



Structural Elucidation

- Candidate material is not from a reputable source and no comparable data exists:
- NMR Experiments (1D & 2D)
  - Proton NMR (HNMR)
  - Carbon NMR (CNMR)
  - Correlation Spectroscopy (COSY)
  - Heteronuclear Single Quantum Coherence (HSQC)
  - Heteronuclear Multiple Bond Correlation (HMBC)
- MS Interpretation
  - EI – Fragmentation
  - DART-TOF – Exact mass and fragmentation
- Salt Form Determination



Monographs:

The Drug Enforcement Administration's Special Testing and Research Laboratory generated the following monographs using structurally confirmed reference materials. These monographs are intended to be used for the verification of acquired reference materials. Monographs are being uploaded as they are technically reviewed and approved for publication. In addition, links to monographs authored by Forensic Drug Review and the Center for Forensic Science Research and Education (CFSRE) are provided below. For those monographs that refer to a TLC method number, please click on the TLC Systems link for more information.

For updates on when new monographs are uploaded, follow us on Twitter. Follow @swgdrug

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

Common Name ▼	Other Names ▼	Mass ▼	MS Base Peak ▼	Date ▼
A796,260	{1-[2-(morpholin-4-yl)ethyl]-1H-indol-3-yl}(2,2,3,3-tetramethylcyclopropyl)methanone	354	100	12-28-12
A834,735	[1-(tetrahydropyran-4-ylmethyl)-1H-indol-3-yl]-(2,2,3,3-tetramethylcyclopropyl)methanone; [1-(tetrahydro-2H-pyran-4-methyl)-1H-indol-3-yl]-(2,2,3,3-tetramethylcyclopropyl)methanone	339	242	05-05-14
A836,339	N-[(2E)-3-(2-methoxyethyl)-4,5-dimethyl-1,3-thiazol-2(3H)-ylidene]-2,2,3,3-tetramethylcyclopropanecarboxamide	310	213	12-16-13
AB-001	JWH-018 adamantyl analog; 1-pentyl-3-(1-adamantoyl)indole; (1-phenyl-1H-indol-3-yl)(tricyclo[3.3.1.13,7]dec-1-yl)methanone	349	214	12-16-13
AB-CHMICA	N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(cyclohexylmethyl)-1H-indole-3-carboxamide	355.5	240	12-07-16
AB-CHMINACA	Monograph provided by Forensic Drug Review	356.5	241	07-22-14
AB-FUBICA	N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-[(4-fluorophenyl)methyl]-1H-indole-3 carboxamide; N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-indole-3-carboxamide	367.4	109	09-26-16
AB-Fubinaca	N-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1H-indazole-3-carboxamide	368	109	07-12-13
AB-Fubinaca Isomers	Monograph provided by Forensic Drug Review	368	109	06-30-15
AB-Fubinaca 2-Fluorobenzyl Isomer	N-[(2S)-1-amino-3-methyl-1-oxobutan-2-yl]- 1-[(2-fluorophenyl)methyl]-1H-indazole-	368	253	03-24-

SWGDRUG Monographs

- General Information
  - *IUPAC Name*
  - *CFR*
  - *CAS*
  - *Synonyms*
  - *Source*
  - *Appearance*
  - *Kovat's Index*
  - *UV_{max}*
- Chemical and Physical Data
  - *Form*
  - *Chemical Formula*
  - *Molecular Weight*
  - *Melting Point*
- Additional Resources
  - *Article citations*
- Qualitative Data
  - *Sample preparation*
  - *Instrument parameters*
  - *Analytical observations for each technique (if necessary)*

✓ ***NMR***
✓ ***GC-MS***
✓ ***FTIR***

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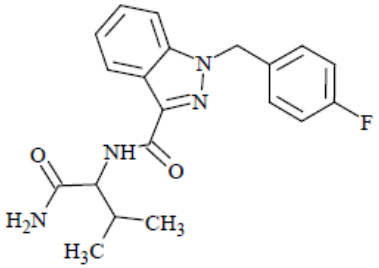
Example

AB-FUBINACA **Latest Revision: July 12, 2013**



1. GENERAL INFORMATION

IUPAC Name:	*N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indazole-3-carboxamide
CFR:	Not Scheduled (7/2013)
CAS#:	1185282-01-2
Synonyms:	N/A
Source:	DEA Reference Material Collection
Appearance:	White powder
Kovat's Index:	Pending
UV_{max} (nm):	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{20}H_{21}FN_4O_2$	368	166.3

3. ADDITIONAL RESOURCES

Uchiyama, N; Matsuda, S; Wakana, D; Kikura-Hanajiri, R; Goda, Y. New cannabimimetic indazole derivatives, *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-pentyl-1*H*-indazole-3-carboxamide (AB-PINACA) and *N*-(1-amino-3-methyl-1-oxobutan-2-yl)-1-(4-fluorobenzyl)-1*H*-indazole-3-carboxamide (AB-FUBINACA) identified as designer drugs in illegal products. *Forensic Toxicol.* **2013,** *31* (1), 93-100.

SWGDRUG Future Directions

- SWGDRUG meetings:
  - Core committee (national & international)
  - DEA – financial support
- Provide resources:
  - Recommendations and supplemental documents
  - Libraries and monographs
- Dissemination
  - www.swgdrug.org
- Support the development of internationally accepted minimum standards for the analysis of seized drugs (OSAC)

SWGDRUG Core Committee

- DEA – Scott R. Oulton (Chair)
- SAFS – Christian Matchett (Vice Chair)
- AAFS – Dr. Sandra Rodriguez-Cruz[1]
- MAFS – Karen Bowen
- MAAFS – Juli Cruciotti
- NEAFS – Tiffany Ribadeneyra
- NWAFS & CAC – Dr. Sandra Sachs
- SWAFS – Roger Schneider
- Educators – Dr. Eric Person and Dr. Ruth Smith

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[1]non-voting

SWGDRUG Core Committee

- ASCLD – Linda Jackson
- ASTM – Agnes Winokur
- FBI – Dr. Jason Brewer
- NIST – Dr. William Wallace
- AFSN/IDWG – Dr. Angeline Yap Tiong Whei
- AICEF – Dr. Adriano Maldaner
- Australia – Catherine Quinn
- Canada – Richard Laing
- ENFSI – Dr. Michael Bovens
- UNODC – Dr. Conor Crean

Thank You!

www.swgdrug.org

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