Authentication of Reference Materials

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Topics

- Reference Material Sources
- Authentication Process
- Monographs
- Contact Information

Where do DEA Reference Materials come from?

- Purchased from commercial sources
- Synthesized in-house

Authentication of Reference Materials

Why??

1. Verify structure of the Reference Material (RM)

2. Determine the purity of the RM

Purity Determination

- Quantitative Nuclear Magnetic Resonance (NMR)
  - Use a NIST traceable internal standard
  - Multiple analyses in order to establish an uncertainty value
  - Material must be ≥98.0% for quantitative reference materials & ≥90.0% for qualitative reference materials

Purity Determination

- Chromatography
  - Gas Chromatography/Flame Ionization Detector (GC/FID)
  - Liquid Chromatography/Photodiode Array Detector (UPLC/PDA)
  - Capillary Electrophoresis (CE)
- Differential Scanning Calorimetry
  - Also provides Melting Point data
- Thermogravimetric Analysis (TGA)
  - Water of Hydration

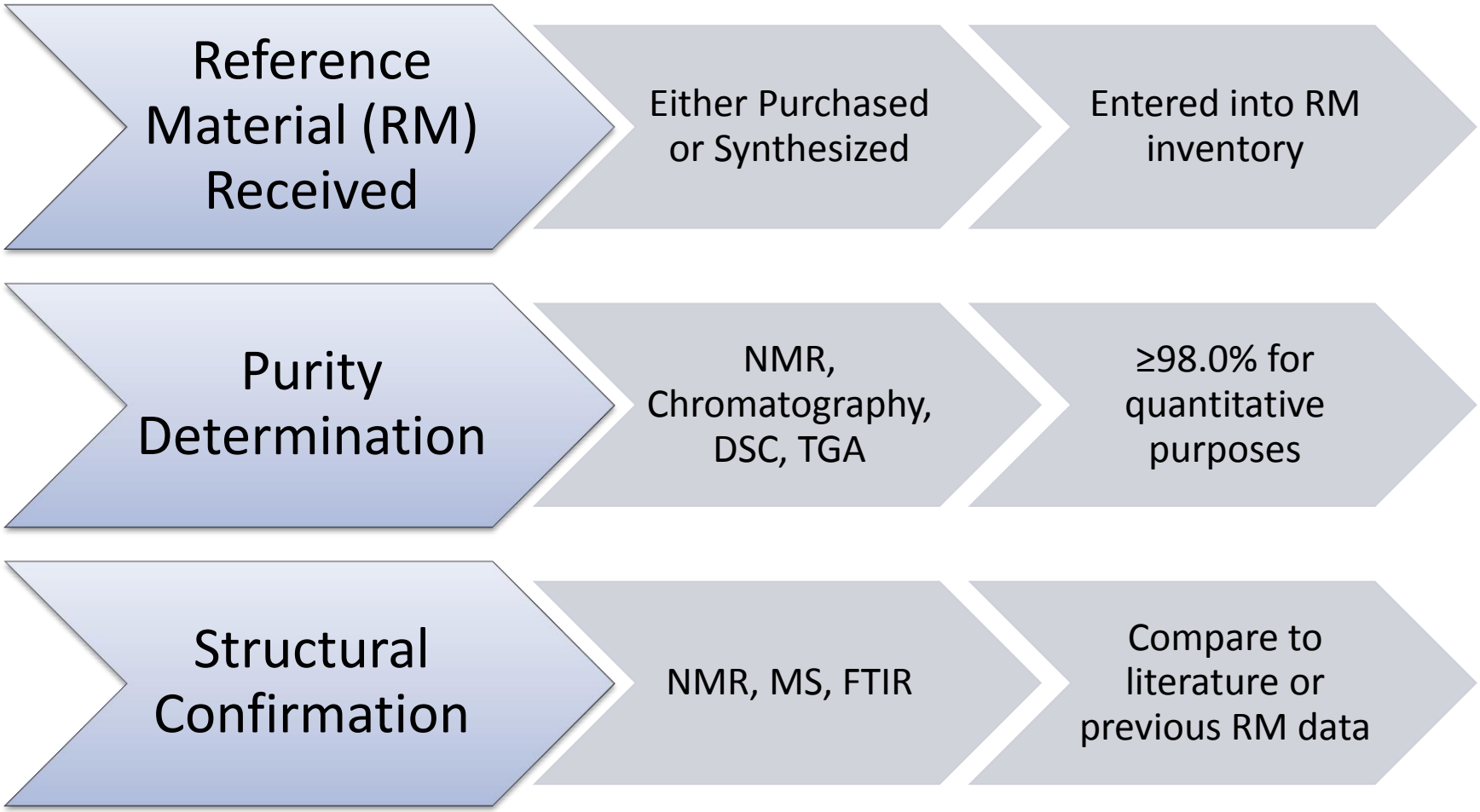
Structural Confirmation

- Required:
  - NMR
  - Gas Chromatography/Mass Spectrometry (GC/MS)
  - Infrared Spectroscopy (FTIR)
- As needed:
  - Polarimetry/CE for isomer determination
  - Microcrystalline tests/Optical crystallography

Structural Confirmation

- Data from identification techniques are compared to:
  - Instrumental Data of Drug Analysis (IDDA)
  - Clarke's Analysis of Drugs and Poisons
  - Peer reviewed articles
  - Previous lots of reference materials

Authentication Process Recap



Compare to literature or previous RM data?

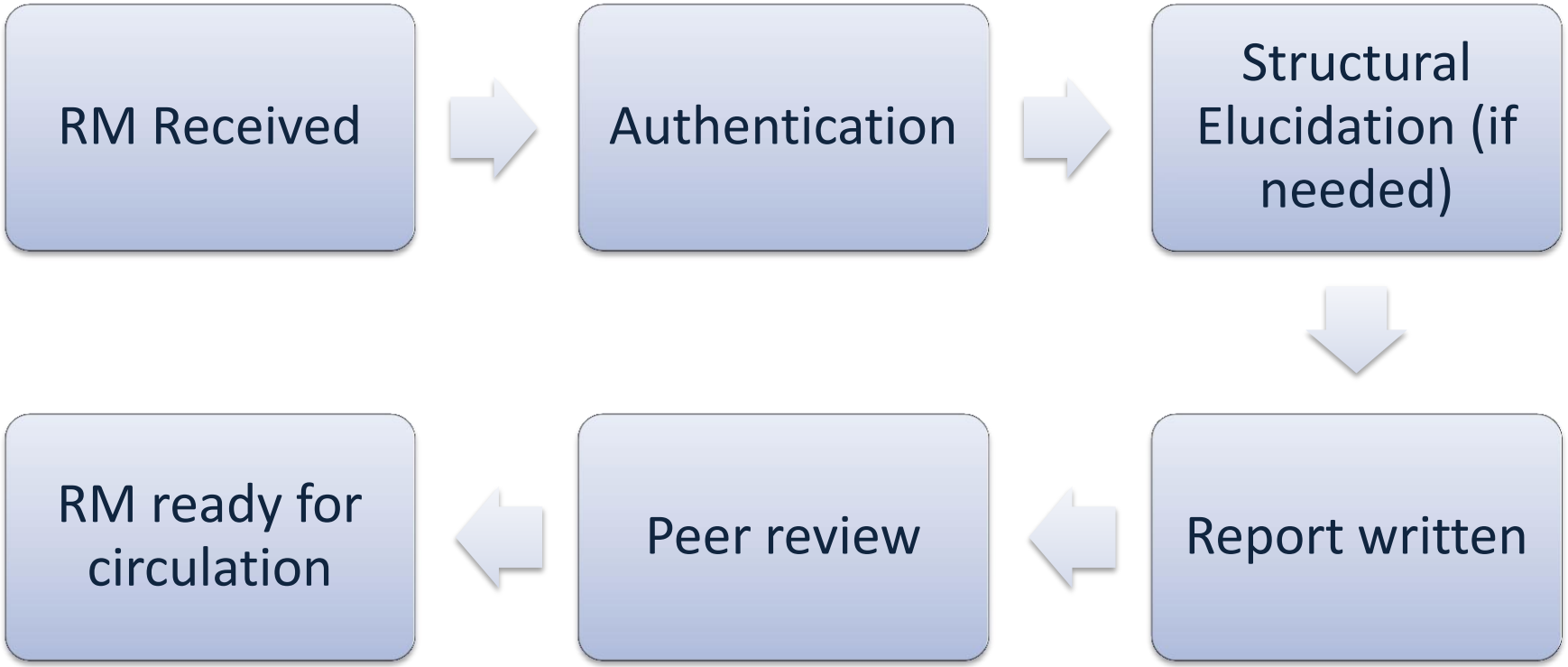
What happens when there is no previous data for comparison?

Structural Elucidation

Structural Elucidation

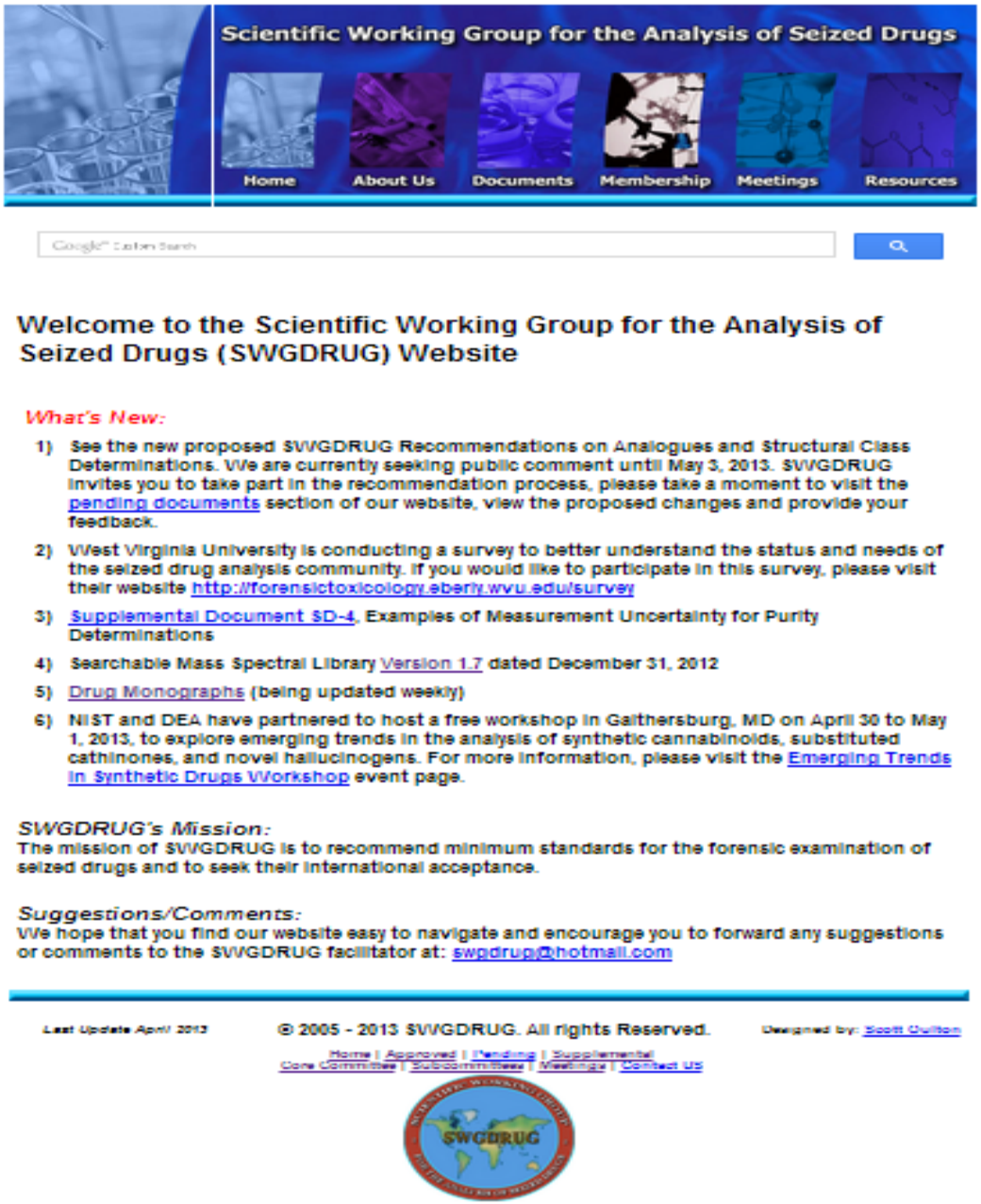
- NMR Experimentation (1D & 2D)
  - Proton NMR (HNMR)
  - Carbon NMR (CNMR)
  - Correlation Spectroscopy (COSY)
  - Heteronuclear Single Quantum Coherence (HSQC)
  - Heteronuclear Multiple Bond Correlation (HMBC)
- MS Interpretation

Authentication Process Recap



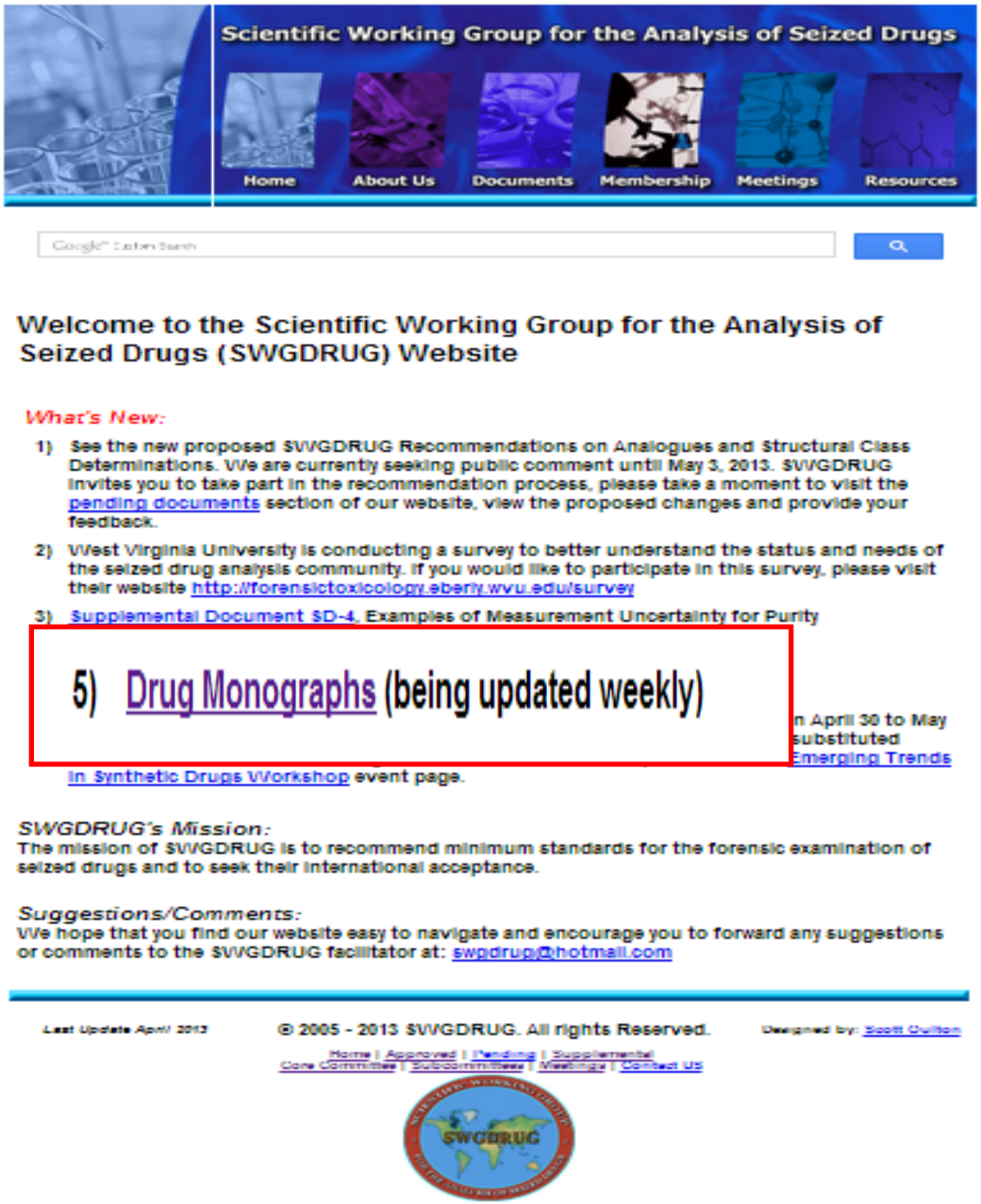
How can DEA assist other forensic laboratories?

- Provide spectra
  - MS & IR data
- Provide drug monographs for SWGDRUG



SWGDRUG MONOGRAPHS

www.swgdrug.org



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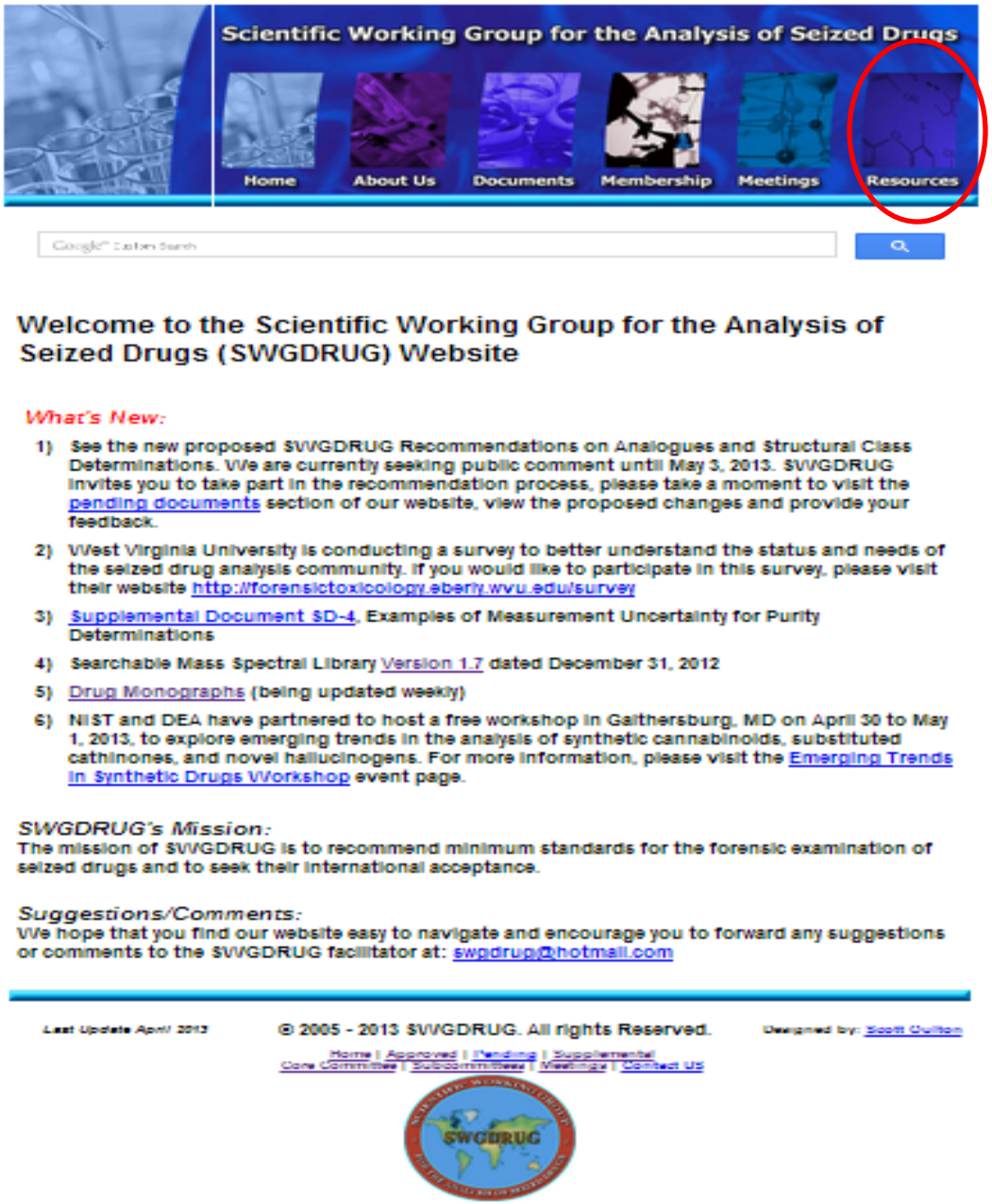

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Welcome to the Scientific Working Group for the Analysis of Seized Drugs (SWGDRUG) Website

SWGDRUG MONOGRAPHS

www.swgdrug.org

Monographs:

The following monographs contain detailed information and analytical data for reference materials which have been analyzed, verified, and authenticated by the Drug Enforcement Administration Special Testing and Research Laboratory. These monographs may be used for the verification of acquired reference materials and for the identification of drug materials (subject to laboratory policy). Monographs are being uploaded as they are peer reviewed and approved for publication.

Google™ Custom Search

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	Date
A796,260	{1-[2-(morpholin-4-yl)ethyl]-1H-indol-3-yl}(2,2,3,3-tetramethylcyclopropyl)methanone	12-28-12
4AcODMT	4-AcO-DMT; psilacetin; O-acetylpsilocin	03-18-13
AKB-48	APINACA; N-adamantyl-1-pentylindazole-3-carboxamide; N-adamantyl-1-pentyl-1H-indazole-3-carboxamide	12-07-12
5-Fluoro-AKB-48	5F-APINACA; APINACA 5-Fluoropentyl analog; 5F-AKB-48	02-08-13

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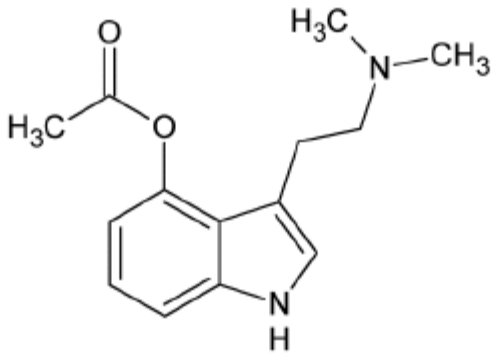

4-Acetoxy-N,N-dimethyltryptamine Latest Revision: March 18, 2013

1. GENERAL INFORMATION

IUPAC Name:	3-[2-(Dimethylamino)ethyl]-1*H*-indol-4-yl acetate
CFR:	Not Scheduled (3/2013)
CAS #:	92292-84-7
Synonyms:	4-AcO-DMT; psilacetin; *O*-acetylpsilocin
Source:	DEA Reference Material Collection
Appearance:	Off-white powder (oxalate)
Kovat's Index:	Pending
UV_{max}:	Not Determined

2. CHEMICAL AND PHYSICAL DATA

2.1 CHEMICAL DATA

Form	Chemical Formula	Molecular Weight	Melting Point (°C)
Base	$C_{14}H_{18}N_2O_2$	246	Not Determined
Oxalate	$C_{14}H_{18}N_2O_2 \cdot C_2H_2O_4$	336	144.2

Contain:

- General Information
- Chemical and Physical Data
- Additional Resources
  - Links to websites
  - Article references
- Qualitative Data
  - Spectra for NMR, MS, & IR
  - Sample preparation and Instrumental conditions used
  - Any analytical observations during data collection

Contact Information

Questions regarding:

- Reference Materials:
  - DEALabRefMaterials@usdoj.gov
- SWGDRUG Monographs:
  - swgdrug@hotmail.com

Thank You