SWGDRUG Meeting Minutes
St. Louis, MO
June 12-15, 2017

Core Committee Members (Present)
Scott R. Oulton, Chair, Drug Enforcement Administration
Christian Matchett, Vice-Chair, Southern Association of Forensic Scientists
Sandra Rodriguez-Cruz, Secretariat, Drug Enforcement Administration
Michael Bovens, European Network of Forensic Science Institutes
Conor Crean, United Nations Office on Drugs and Crime
Garth Glassburg, American Society of Crime Laboratory Directors
Richard Laing, Health Canada
Adriano Maldaner, Iberoamerican Academy of Criminalistics and Forensic Studies
Catherine Quinn, Victoria Forensic Science Centre, Australia
Tiffany Ribadeneyra, Northeastern Association of Forensic Scientists
Sandra Sachs, California Association of Criminalists
Roger Schneider, Southwestern Association of Forensic Scientists
Agnes Winokur, Drug Enforcement Administration and ASTM International
Angeline Yap, Asian Forensic Sciences Network

Core Committee Members (Not Present)
Eric Person, California State University, Fresno

Guests
Toshinori Ando, Japan
Shigetoshi Aoyama, Japan
Karen Bowen, Midwestern Association of Forensic Scientists
Dr. Anne Slaymaker, Note Taker, Drug Enforcement Administration
Dr. Ruth Waddell Smith, Michigan State University
Dr. William Wallace, National Institute of Standards and Technology
Juli Cruciotti, Mid-Atlantic Association of Forensic Scientists

MONDAY – June 12, 2017

Welcome and Opening Remarks – Mr. Scott Oulton

- SWGDRUG Chair Mr. Scott Oulton opened the meeting by welcoming the committee members and thanking Secretariat Dr. Sandra Rodriguez-Cruz for coordinating the meeting and all travel arrangements. He also welcomed the guests in attendance (Ms. Karen Bowen, Dr. Ruth Waddell Smith, Dr. Bill Wallace, Dr. Anne Slaymaker, Mr. Shigetoshi Aoyama, and Mr. Toshinori Ando). Mr. Oulton discussed the current SWGDRUG Core Committee vacancies (MAFS, Educator, NIST, FBI, private laboratory, and other International representation).

- Mr. Oulton discussed SWGDRUG funding and continuous funding by DEA.

- Mr. Oulton discussed OSAC activities during the last year and SWGDRUG's role within the seized drugs community. SWGDRUG will continue providing resources to the community and revising Recommendations, as needed.

- This year marks the 20th anniversary of SWGDRUG. Unfortunately, an in-person reunion was not possible due to conflicts/travel costs.

Discussion Items and Goals for the Week – Mr. Scott Oulton and Mr. Christian Matchett

- Method Validation – The full committee discussed method validation, the overall analytical scheme, and the A/B/C technique categorization. It was noted that any discussion regarding method validation will be interrelated with acceptance criteria. Discussion included possible revisions to current SWGDRUG Recommendations and continuing the development of supplemental document (SD-7) to provide clear guidance to laboratories. Further discussion included future ANAB requirements and their interpretation by different disciplines. Dr. Bovens stated that expert knowledge and competence of the analyst is key and must be a part of any minimum recommendations made. Further discussion tabled for sub-committee break-out.

- The drafting of a Primer on A-B-C categorization (possible SD-8) was discussed. Dr. Eric Person had provided committee with preliminary draft/outline. Core committee members agreed on the need for such document to clarify original intent of techniques' classifications within the scope of analysis scheme design.

- SWGDRUG Glossary – Revisions to the glossary were discussed, including addition of the terms "discriminating power", "analytical scheme", etc. The use of the term "uncorrelated" and its removal from E2329 was also discussed.

- Pharmaceutical Identifiers – Core committee members discussed pharmaceutical identifiers and their SWGDRUG classification under Category B. Various members expressed interest in lowering classification to a Category C, while others would prefer classification to remain unchanged. It was remarked that this discussion reiterates the need to clarify the purpose of Category A-B-C techniques within the design of the analytical scheme.

- Dr. Rodriguez-Cruz shared the original 1997 TWGDRUG document language with members of the Method Validation sub-committee for possible reincorporation into the current Recommendations.

- The consideration of macro/microscopical testing for cannabis as "uncorrelated" techniques was briefly discussed.
- Harmonization of SWGDRUG recommendations and ASTM documents – Mr. Oulton stated that SWGDRUG's mission will be to continue to provide the Recommendations as a free

resource via the SWGDRUG website. Any applicable changes brought about via OSAC and ASTM discussions may be incorporated into the SWGDRUG recommendations. Most importantly, harmonization needs to happen to ensure that documents don't contradict one another.

- The topic of acceptance criteria for qualitative tests was also briefly discussed. It will also be part of discussions relating to method validation.

- Other discussion topics:

    - Dr. Bovens and Ms. Ribadeneyra expressed interest in developing a spreadsheet uncertainty calculator to supplement SD-6.

    - Dr. Yap suggested the following additions to the SWGDRUG website:

        - Adding hyperlinks to additional databases.

        - Including a list of compounds which are thermally labile or degrade on GCMS. She provided an example of the recent NBOH compound which degrades into the corresponding 2C compound within the heated GC injection port.

        - Making the monograph page more user-friendly by making it sortable by base peak, etc.

Qualitative Method Validation Sub-Committee Update (Ms. Catherine Quinn)

- Ms. Quinn provided a status update for the sub-committee. This sub-committee originally split into two groups – one working on revisions of Part IVB and the other drafting a supplemental document containing examples of qualitative method validation (GC-MS, IR, color test). In this meeting, she would like to first discuss the SWGDRUG position regarding the definition of analytical scheme, ABC categorization, discriminating power, etc. prior to continuing work within the method validation sub-committee.

- Mr. Matchett confirmed the sub-committee's goal for the week and verified it had enough members to achieve goals effectively.

Update from NCFS, OSAC, FSSB (SAC – Chemistry and Seized Drug) – Mr. Scott Oulton and Dr. Sandra Rodriguez-Cruz

- Mr. Oulton – The National Commission on Forensic Science has ended and Attorney General Jeff Sessions will be bringing on a science advisor before moving forward. There has been discussion about the future of OSAC and what version 2.0 would look like; this discussion is on-going.

- Dr. Rodriguez-Cruz – One of the main difficulties OSAC has faced has been to get all parties involved to have an understanding of the documents. There needed to be a learning/adjusting of perspective from all disciplines. The document acceptance process has been cumbersome. So far there are two documents posted to the registry (E2329 and E2548). The Seized Drugs subcommittee is working on a GC-MS acceptance criteria document (SWGDRUG members Dr. Sachs and Dr. Waddell Smith are also contributors). If the GC-MS acceptance criteria document does not proceed out of OSAC, it can be made available to community via SWGDRUG.

ENFSI-DWG Update (Dr. Michael Bovens)

- Dr. Bovens reviewed the topics covered at ENSFI-DWG meeting (May 2017). The topics discussed included a focus on increasing efficiency through automatization, increasing seizures on pre-precursors on NPS, and the launch of the NPS data hub (www.nps-datahub.com) to gather international analytical data of NPS compounds. The NPS data hub is NMR based with some MS and IR data and is a collaboration between NIST (Katrice Lippa, Aaron Urbas), DEA (Charlotte Corbett), and BKA and Sci Formation (Felix Rudolphi software company).

- Mr. Oulton questioned the usefulness of creating more databases and duplicating efforts and suggested that coordination be done to compile all the data into one place. The group consensus was that one database for forensic science community as a whole should be the goal.

- Dr. Bovens also discussed various tools for nomenclature of NPS including the following.
  - https://chemicalize.com/welcome
  - http://opsin.ch.cam.ac.uk
  - https://cactus.nci.nih.gov/chemical/structure

- Dr. Bovens discussed the lack of an open source for locating CAS numbers for new NPS. He queried the committee to see if anyone was aware of one beyond SciFinder. Dr. Wallace suggested using InChIKey instead of CAS numbers, as the latter are not generated until after publication and are not always unique. InCHIkeys are unique, can be created on demand, and are open source. He also stated that CAS numbers are the property of ACS, so there's no free open source database listing them. Dr. Bovens commented that some national legislation processes need CAS numbers. Dr. Wallace did suggest ChemSpider, as NIST has found it to be fairly reliable; however, he did caution users regarding instance of erroneous CAS numbers for some stereoisomers.

- Additional ENFSI-DWG meeting updates provided by Dr. Bovens included:

  - Fentanyl issues in Europe (not as frequent as US/Canada).

  - Discussion on the increased use of NMR for quantifications.

- A recent ENFSI-DWG proficiency test which required structural elucidation of NPS compound.

- A court testimony workshop.

- Discussion of implementation of the ENSFI-DWG Sampling for Quantitative Analysis guidelines by DEA and other European forensic drug laboratories.

- Creation of a new ENFSI-DWG sub-committee to develop a Best Practice Manual for Seized Drug Analysis.

- Dr. Bovens also provided an update from the ENFSI-DWG Chemometrics sub-Committee and its goal to provide guidance on how to process a dataset using chemometric methods to answer a relevant forensic question. The sub-committee is striving to have deliverables within the next two years. Mr. Laing questioned if data could be input from outside sources (other laboratories) and the software used to make comparisons? It depends on the nature of the data. For drug profiling, it has been demonstrated that reference material and sample data must be collected on the same instrument/method for comparison; unless standard samples are run in both labs and correction factors applied.

ASFN-IDWG Update (Dr. Angeline Yap)

- The 2017 AFSN meeting (www.afsn2017.sg) will be held in Singapore in September 2017.

- Dr. Yap provided an overview of the drugs of abuse trends from 13 participating laboratories (11 countries).

- Dr. Yap also discussed timeline of NPS compounds and legislation in Singapore since 2011. She also discussed the overall analytical scheme utilized at her laboratory and new procedures implemented in response to a recent incorrect identification of NBOH due to degradation in the GC inlet. A second non-GC test is now required in order to identify all new NPS.

- Dr. Yap provided a demonstration of the Japanese database, a data search system for NPS. The database contains >700 compounds, chemical information, and GC-MS, LC, LC-MS, and IR spectral data.

    - Dr. Rodriguez-Cruz asked about procedures used by analysts to decide if the data obtained is sufficient for identification? Dr. Yap relayed the current GC-MS acceptance criteria in place in the laboratory. For example, for cases when no molecular ion is apparent, another technique must be used to obtain such information.

Fentanyl/Opioid Analytical Issues (Canada/US – Mr. Richard Laing, Ms. Agnes Winokur)

- Mr. Laing provided an overview of the fentanyl and related compounds situation in Canada. Overall, a decrease in cannabis has been observed, with an increase of non-cannabis samples. In 2015, fentanyl analogues began being identified in significant numbers and they are no longer seen as diverted pharmaceuticals. The majority of fentanyl analogues are being seen in western Canada with 30 samples of carfentanil analyzed in 1 month.

- Mr. Laing also gave an overview of an industrial hygiene survey conducted due to the increasing number of fentanyl and TATP submissions. The results of this survey found that the analysts' exposure level is very low if good laboratory practice is used. Current safety protocols now suggest using N95 masks at the bench and analyzing high-purity samples in a fume hood. The biggest exposure risk was found to be through inhalation as it takes 4 – 6 minutes to get a dosing through skin absorption.

    - The group discussed how agents are being protected and their safety in the field without the engineering controls that a laboratory has. The very low purity levels and lack of adverse incidents should be some reassurance to agents.

    - Mr. Laing will forward copy of study to members.

- Ms. Winokur provided an overview of the fentanyl issue in the US and Florida. She emphasized the need to communicate between agents, analysts, medical examiners, etc. The US has seen a drastic increase in fentanyl related seizures since 2012 in all forms, with carfentanil being seen in several states. The fentanyl outbreak in 2006 was tracked back to a single laboratory in Mexico. The current outbreak, however, is being sourced from China by many individuals/organizations. DEA, AAFS, and the CDC are all working on communication and safety efforts. She also discussed the challenges in analyzing and reporting these substances.

NIST & SWGDRUG MS Library Project Update (Dr. William Wallace)

- The mass spectrometry group at NIST consists of 19 federal employees and 13 contractors, of which approximately 1/3 work on GCMS; 1/3 work on LCMS; and 1/3 work on software. A new library is issued every 3 years and all money spent on the purchase of libraries is directly spent on further library development. Since the 1990s, every spectrum in the library is fully evaluated. There are over 267,000 unique compounds in the current electron-ionization library and almost 14,000 compounds in the electrospray ionization tandem MS library.

- Dr. Wallace discussed two software tools available: AMDIS (Automated Mass Spectral Deconvolution and Identification System) for the deconvolution of gas chromatograms and the NIST MS Interpreter for the thermochemical prediction of electron-ionization fragmentation patterns. Both as available free at chemdata.nist.gov.

- NIST recently conducted an evaluation of the SWGDRUG mass spectral library. All errors have been corrected and many entries from the SWGDRUG library were incorporated into the NIST2017 electron-ionization library (released June 6, 2017). The SWGDRUG library will continue to be reviewed by NIST on a quarterly basis.

- Current projects at NIST were discussed including working with DEA's Special Testing and Research Laboratory and Virginia Department of Forensic Sciences to develop a DART library.

- He also provided an overview of the newly developed NIST hybrid search function in the MS Search software for structurally similar compounds as opposed to spectrally similar.

- Mr. Oulton discussed posting the NIST tools on the SWGDRUG website.

Update on next CLIC meeting (Mr. Roger Schneider)

- The 2017 CLIC meeting will be held in Phoenix September 5-9, 2017. The workshop is on Considerations of Spectral Search Algorithms.

ASTM Update (Ms. Agnes Winokur)

- Ms. Winokur provided an overview of the standards documents that have been approved by ASTM and provided an update on the status of those that are in-progress.

TUESDAY – June 13, 2017

Full core committee discussion

- The following terms were discussed. Future revisions to these terms or clarifications will be incorporated in the SWGDRUG glossary:

    - Analytical Scheme: To be also defined within Part IIIB

    - Discriminating Power: Potential removal of this terminology discussed. Committee agrees rationale behind categorization of techniques should be clarified.

    - Correlated/Uncorrelated: Potential removal of this terminology discussed and use of "orthogonal" instead. Committee agrees to clarify intent: for analysts to use different techniques with differing principles during identification of a substance.

    - Error (Type I and II): Committee agrees to use the terms false positive and false negative instead.

Sub-Committee Break-out Sessions

- Sub-committee meetings until the end of the day.
- Recommendations Part IIIB: Ms. Catherine Quinn, Dr. Conor Crean, Ms. Agnes Winokur, Mr. Richard Laing, Dr. Ruth Waddell Smith, Dr. Angeline Yap, Dr. Rodriguez-Cruz.

- Revisions to SD-6: Ms. Tiffany Ribadeneyra, Dr. Michael Bovens, Dr. Rodriguez-Cruz

- Public Communication: Ms. Karen Bowen, Mr. Christian Matchett

- SD-7 – Qualitative Method Validation Examples: Dr. Sandra Sachs, Ms. Juli Cruciotti, Mr. Garth Glassburg, Dr. Adriano Maldaner, Dr. Anne Slaymaker, Dr. William Wallace, Mr. Roger Schneider, Dr. Rodriguez-Cruz.

- Website: Mr. Scott Oulton

WEDNESDAY – June 14, 2017

- Mr. Matchett provided an overview of the public communication project. A SWGDRUG bulletin is being developed and will be sent to all SWGDRUG core committee members after each meeting. Committee members are then to forward it to their respective organizations. SWGDRUG will not maintain a mailing list for this, and will alternatively post it on the website.

- Mr. Oulton provided an update on the revisions made to the SWGDRUG monographs webpage. Sortable nominal mass and MS base peak columns have been added. NO other columns will be added at this time. A Google search bar is still available above the list for text searching of the monographs.

Assessment of Error Rates in Seized Drug Laboratories (Dr. Sandra Sachs and Dr. Sandra Rodriguez-Cruz)

- Dr. Sachs presented slides summarizing the qualitative error rate evaluations done at DEA, Oakland PD, and the Kern Regional Crime Laboratory, using PT data, re-analysis thru QA program, and casework re-analysis, respectively. An abstract has been submitted to the 2017 NIST Error Management Symposium.

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THURSDAY – June 15, 2017

- After discussion and unanimous vote by core committee members, Ms. Juli Cruciotti and Dr. William Wallace were confirmed as new members of the SWGDRUG core committee.

- Mr. Oulton discussed the current core committee vacancies. With Mr. Glassburg's retirement, there is now an ASCLD vacancy. In the future, SWGDRUG will also be considering members representing the Mediterranean region, a private company, South Africa, and the UK.

Sub-committee Updates

- SD-6 Calculator: Ms. Ribadeneyra provided overview of the SD-6 Calculator for net weight extrapolation uncertainty calculations. Mr. Glassburg suggested the calculator and other tools can be advertised via webinars and training at regional meetings. Dr. Rodriguez-Cruz noted that validation of the calculator should be done prior to posting the spreadsheet on the website. Ms. Ribadeneyra will send a draft version out to the committee for review.

- SD-6 Revisions: Dr. Bovens presented new language added to example B within SD-6. A statement clarifying the rationale behind the calculation of bags to be selected using hypergeometric distribution. Dr. Bovens and Ms. Ribadeneyra will finalize the document and send to Dr. Rodriguez-Cruz for dissemination and review by sub-committee.

How to Build a Scheme/Parent Document Revisions

- Ms. Quinn provided an overview of the proposed revisions to Part IIIB of the recommendations. The proposed changes avoid descriptions based on "discriminating power" and instead describe the rationale behind the categorization of techniques. Revisions are expected to minimize misinterpretation of recommendations and encourage critical thinking by the analysts when building their analytical schemes.

- Group discussion was held on whether two samplings is a requirement or a suggestion. Mr. Glassburg noted that the recommendations allow for hyphenated techniques to count as two tests, so he inquired as to how the sampling requirement would affect that recommendation. Subject was reserved for future discussions.

- A draft for a new supplemental document was presented: "Construction of An Analytical Scheme". The objective of the document is to present different examples of analytical scheme designs for different laboratory/jurisdiction scenarios. The examples emphasize how different tests in a scheme must be combined to answer the question at hand, while simultaneously addressing all applicable limitations.

Qualitative Method Validation Examples Supplemental Document

- SD-7 (Examples of Qualitative Method Validation) Update: Dr. Sachs summarized the sub-committee's work and discussions but noted that document is not mature enough for core committee discussion. The sub-committee recommends the document should provide guidance for validation of new qualitative methods as well as guidance to demonstrate valid methodology retroactively. The SD will discuss method validation approaches that include producing method validation documentation for each compound analyzed or alternate ways to use an approved validated method to assess a new compound. .

- The sub-committee notes that method validation requirements should emphasize that the onus is on the laboratory to critically evaluate their methods, SOPs, and established acceptance criteria, to determine the extent of method validation necessary to ensure accurate and reliable results.

- The following validation performance characteristics are being considered:

    - *Selectivity* – to be the minimum testing recommended by SWGDRUG; other characteristics may be evaluated based on laboratory needs and scope of individual methods.
    - *Limit of detection*
    - *Precision* – to be based on the scope of the method and laboratory policies. For example, day-to-day reproducibility evaluation not needed if laboratory policy requires contemporaneous analysis of positive controls.
    - *Sensitivity* – true positive rate
    - *Specificity* – true negative rate
    - *Accuracy*

Additional Discussion Items

- Part IVA of the Recommendations will need revision as a result of ongoing Part IIIB changes, as well as to clarify meaning of phrase "same analytical conditions". Core committee members are invited to comment on this after the meeting.

- X-ray diffractometry was moved under Category B and X-ray crystallography was added to the list of Category A techniques. Supercritical fluid chromatography and UV-Vis (full spectrum) were also added under Category B. Dr. Maldaner's commented on a future proposal suggesting the inclusion of some electrochemical techniques.

- Mr. Laing asked members to opine on the analyst's responsibility to prove sample identity for instances of theoretical isomers that are not possible or available. This is seen as an issue affecting the entire seized drug community, but no guidance is available. Dr. Yap shared how HSA Singapore has addressed these situations by presenting an example of the evaluation of the possible isomers of dibutylone.

Closing Remarks

- Mr. Oulton emphasized SWGDRUG's important role in the forensic science community and ensured that documents and resources will continue to be provided in an effective and timely matter.

- Mr. Oulton requested sub-committee members to continue offline work after the meeting so that an updated version of the SWGDRUG Recommendations can be forwarded for public comments before the end of the year.

    - Ms. Ribadeneyra will work on the revisions to SD-6 and calculator and send to Dr. Rodriguez-Cruz for dissemination and review by the core committee.

    - Ms. Quinn's sub-committee will continue revising Past IIIB and drafting of the new SD containing analytical scheme examples.

    - Dr. Rodriguez-Cruz will work on incorporating comments received from OSAC/ASTM/NIST into Part IIIA (sampling) of the Recommendations.

    - Dr. Sandra Sachs and sub-committee will continue work on SD containing three examples of qualitative method validation.

    - Mr. Oulton will draft introduction for Part IIIB discussing the need for critical thinking when designing analytical schemes.

- Next meeting is tentatively scheduled for June 2018. Future meetings may be hosted by domestic members/laboratories on a rotating basis. Annual meeting may be increased to five days next year. Positive feedback was received this year after extending meeting by one day. The possibility of having a method validation sub-committee meeting (online/phone) was also discussed.

- Mr. Oulton closed the meeting by thanking the core committee for their hard work this week and to Mr. Matchett and Dr. Rodriguez-Cruz for organizing the annual meeting. He also officially welcomed Ms. Cruciotti and Dr. William Wallace to the SWGDRUG core committee and thanked the guests who participated this week, Ms. Bowen, Dr. Smith, and Dr. Slaymaker.

Sub-Committee Break-out Sessions

- Additional sub-committee meetings until the end of the day.

Minutes respectfully submitted by Dr. Anne Slaymaker.