OPCW

Scientific Advisory Board

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REPORT OF THE SCIENTIFIC ADVISORY BOARD'S WORKSHOP ON CHEMICAL FORENSICS

1. EXECUTIVE SUMMARY

1.1 The OPCW Scientific Advisory Board (SAB) in cooperation with VERIFIN held a workshop,[1] "Chemical Forensics: Capabilities across the Field and the Potential Applications in Chemical Weapons Convention Implementation", from 20 to 22 June 2016 in Helsinki, Finland. The workshop is one of a series intended to inform the report of the SAB on developments in science and technology to the Fourth Review Conference[2] of the Chemical Weapons Convention to be held in 2018. Interest in chemical forensics, and its relevance to the work of the OPCW, has been described through Recommendation 17 of the OPCW SAB's Temporary Working group on Verification.[3]

1.2 Forensic science is defined as the study of traces (remnants of presence and/or activity).[4, 5] These are silent witnesses that need to be detected, seen, and understood to make reasonable inferences about criminal phenomena, investigation or demonstration for intelligence, investigation and court purposes.

1.3 Chemical forensics aims to obtain information from chemical remnants that is relevant to investigative, legal and intelligence questions. Just as fingerprints and DNA can provide unique signatures that can be used to identify individuals, chemical samples can provide distinctive signatures (for example through their impurities

1 Funding for the workshop was provided in part through project III (Science and Technology: Assessment of Developments in Science and Technology) of EU Council Decision (CFSP) 2015/259 dated 17 February 2015. http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=uriserv:OJ.L_.2015.043.01.0014.01.ENG

2 Fourth Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention.

3 Verification, Report of the Scientific Advisory Board's Temporary Working Group (SAB/REP/1/15, dated June 2015). Available at www.opcw.org/fileadmin/OPCW/SAB/en/Final_Report_of_SAB_TWG_on_Verification_-_as_presented_to_SAB.pdf

4 Forensic science on trial. Proceedings of the Plenary presentations from the 20th ANZFSS International Symposium on the forensic sciences, Sydney 2010; *Australian Journal of Forensic Sciences*, 2011, 43:2-3, 89-103. http://www.tandfonline.com/toc/tajf20/43/2-3

5 C. Roux, F. Crispino, O. Ribaux; *Current Issues in Criminal Justice*, 2012, 24(1), 7-24. http://www.austlii.edu.au/au/journals/CICrimJust/2012/16.pdf

and/or isotopic ratios) that might reflect how and where they originated.[6] Combining this type of information with other data sources could provide information that can be used to ascertain the origins of a chemical agent or reconstruct the event in which it has been used. The workshop was intended to review the field and understand how chemical forensic (and other forensic methods) might be applicable to Chemical Weapons Convention investigations. Experts in chemical and forensic analysis from a broad range of fields were assembled to share experiences and discuss topics, including: investigations of the use of chemical weapons, evidence collection, forensic intelligence, chemical forensics in illegal drug analysis, biomedical sample analysis, and chemical analysis techniques used in other investigative and retrospective analytical applications.

1.4 The workshop was chaired by Dr Christopher Timperley (OPCW SAB Chairperson). Dr Timperley, Dr Jonathan Forman (OPCW Science Policy Adviser and Secretary to the SAB) and Professor Paula Vanninen (VERIFIN) opened the workshop, welcoming the participants and providing an overview of the programme and its intended outcomes.

1.5 From the workshop discussions, the following outcomes are submitted for consideration by the SAB at its Twenty-Fourth Session in October 2016:

(a) Given the information that chemical forensic techniques can bring to investigations, it would be valuable to continue gathering information and understanding capabilities within this field. In this regard, additional workshops or a temporary working group (TWG) could be considered. Participants would include forensic experts, forensic practitioners and OPCW inspectors, to explore how to develop forensic methods and capabilities for Chemical Weapons Convention verification.

(b) Appropriate functions within the OPCW could benefit from cooperative working relationships with organisations and networks of experts relevant to forensics.

(c) Establishing a system for the management of data, including compilation, curation and analytics, is essential for use in a forensic capacity. In a chemical weapons investigation context, requirements (including those of associated infrastructure and support) would need to be defined.

(d) Collection and curation of samples, analytical information and annotation that may not be immediately actionable is advisable. A searchable collection of physical objects and information is valuable for retrospective review. For example, existing compiled data on abandoned chemical weapons and impurity profiles for known synthetic routes to nerve and vesicant agents could serve as a resource to those working in the field of chemical weapons related investigations.

(e) Methods using impurity profiling and isotopic ratio distribution for purposes related to determining responsibility for use of chemical weapons, for

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6 B. Halford. Tracing A Threat; *Chemistry and Engineering News*, 2012, 90(6), 10-15. http://cen.acs.org/articles/90/i6/Tracing-Threat.html

abandoned chemical weapons, or for clandestine chemical weapons production are valuable to develop. The possible profiling of impurities not related to the product, such as solvents, trace metals and inorganic elements, should be considered.

(f) Recent developments in biomedical sampling methods for determining exposure to chlorine were discussed. Consideration should be given to development of biomedical methods for determining exposure to other toxic industrial chemicals that might be used as chemical weapons. Development of Recommended Operating Procedures for the sampling of biomedical materials, and their handling and storage, is valuable in such investigations.

(g) Autonomous systems to support investigations of alleged use of chemical weapons could benefit investigators, in addition to their use for sampling and on-site analysis and in detection systems.

(h) Forensic training will continue to be valuable for enhancing forensic awareness and forensic investigation capabilities.

(i) Workshop participants recognised the value of broader engagement with experts from other disciplines using forensic approaches in which chemistry plays a key role. The Technical Secretariat would benefit from continuing to find such opportunities to share experiences with relevant communities of experts.

2. AGENDA ITEM TWO – Adoption of the Agenda

The workshop adopted the following agenda:

1. Opening of the session
2. Adoption of the agenda
3. *Tour de table* to introduce workshop participants
4. Establishment of a drafting committee
5. Experience and perspectives on investigations related to the use of chemical weapons
    (a) OPCW missions in the Syrian Arab Republic
    (b) OPCW Fact-Finding Mission
    (c) Sampling and analysis and the role of the OPCW Laboratory and the Designated Laboratories
    (d) Lessons learned
6. Chemical forensics and chemical weapons
    (a) Identification and origin of abandoned chemical weapons

(b) Position Specific Isotope Analysis (NMR) of Chemical Agents

(c) Chemical forensics of chemical agents

7. Chemical forensics in law enforcement

(a) On-site forensic investigations and evidence collection

(b) Forensic chemistry, forensic intelligence and illicit drugs

8. Biomedical samples

(a) Forensic toxicology

(b) Biomedical samples in chemical weapons and toxins analysis

(c) TOXI-triage

9. Other attribution analysis

(a) Food safety and toxins

(b) Chemical forensics and art

10. Reconstructing past events

(a) Chemical forensics in archaeology

11. Breakout groups

(a) How can chemical forensics be combined with investigative chemical analysis?

(b) Limitations and required reference materials?

(c) Methodologies with potential for use in CW applications?

(d) Normal samples vs. highly toxic samples?

12. Adoption of the report

13. Closure of the workshop

3. AGENDA ITEM THREE – *Tour de Table* to Introduce Workshop Participants

A *tour de table* was undertaken to introduce the workshop participants. A complete list of participants is contained in the Annex to this report.

4. AGENDA ITEM FOUR – Establishment of a Drafting Committee

A drafting committee of members of the SAB was formed to prepare the draft report of the workshop.

5. AGENDA ITEM FIVE – Experience and Perspectives on Investigations Related to the Use of Chemical Weapons

5.1 The workshop began with a briefing on contingency operations and investigations involving the OPCW, drawing on the past and on-going experiences in the Syrian Arab Republic. The session was moderated by Dr Christophe Curty.

Subitem 5(a): OPCW missions in the Syrian Arab Republic

5.2 Mr Dominique Anelli (a former head of the OPCW Chemical Demilitarisation Branch) provided an overview of the work of the OPCW in Syria. The OPCW has been engaged in a series of (parallel and consecutive) missions in Syria, starting with the United Nations Secretary-General's Mechanism (UNSGM) investigation in 2013.[7] In September/October 2013, the Joint Mission with the United Nations to eliminate Syria's chemical weapons programme began,[8] followed by OPCW activities in Syria to complete the elimination of Syria's chemical weapons production facilities. Reports of the use of toxic chemicals in Syria initiated the Fact-Finding Mission (FFM). A Declarations Assessment Team (DAT) was established to clarify aspects of Syria's declaration to the OPCW. Most recently, the (still ongoing) OPCW-UN Joint Investigative Mechanism (JIM) was tasked to establish facts that may lead to the identification of those responsible for the use of toxic chemicals in the Syrian armed conflict.[9, 10] The JIM is an independent mechanism, that includes seconded OPCW staff and draws on the reports of the FFM.[11,12,13,14]

5.3 Mr Anelli further described OPCWs experiences in verifying the destruction of Syria's former chemical weapons production facilities. There were a total of 27

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7 "United Nations Mission to Investigate Allegations of the Use of Chemical Weapons in the Syrian Arab Republic", United Nations, 12 December 2013. https://unoda-web.s3.amazonaws.com/wp-content/uploads/2013/12/report.pdf

8 For further information see: https://opcw.unmissions.org/

9 First report of the Organisation for the Prohibition of Chemical Weapons-United Nations Joint Investigative Mechanism; United Nations (S/2016/142, dated 12 February 2016). http://www.securitycouncilreport.org/atf/cf/%7B65BFCF9B-6D27-4E9C-8CD3-CF6E4FF96FF9%7D/s_2016_142.pdf

10 Second report of the Organisation for the Prohibition of Chemical Weapons-United Nations Joint Investigative Mechanism; United Nations (S/2016/530, dated 10 June 2016). http://www.un.org/ga/search/view_doc.asp?symbol=S/2016/530

11 Summary Report of the Work of the OPCW Fact-Finding Mission in Syria Covering the Period from 3 to 31 May 2014 (S/1191/2014, dated 16 June 2014). http://www.the-trench.org/wp-content/uploads/2016/01/OPCW-FFM-20140616-1st-Chlorine-investigation-report.pdf

12 Second Report of the OPCW Fact-Finding Mission in Syria, Key Findings (S/1212/2014, dated 10 September 2014): http://photos.state.gov/libraries/netherlands/328666/pdfs/SECONDREPORTOFTHEOPCWFACT-FINDINGMISSIONINSYRIAKEYFINDINGS.pdf

13 Third Report of the OPCW Fact-Finding Mission in Syria (S/1230/2014, dated 18 December 2014). http://www.the-trench.org/wp-content/uploads/2016/01/OPCW-FFM-20141218-3rd-Chlorine-investigation-report.pdf

14 Report of the OPCW Fact-Finding Mission in Syria regarding the incidents described in communications from the Deputy Minister for Foreign Affairs and Expatriates and Head of the National Authority of the Syrian Arab Republic from 15 December 2014 to 15 June 2015 (S/1318/2015/Rev.1, dated 17 December 2015). http://www.the-trench.org/wp-content/uploads/2016/01/OPCW-FFM-20151217-Syria-request-Rev1.pdf

declared sites that included mobile and fixed facilities; 24 of which have currently been destroyed.

Subitem 5(b): OPCW Fact-Finding Mission

5.4 Mr Lennie Phillips (a Team Leader in the OPCW FFM) briefed the workshop on the investigations of incidents reported in the Syrian Governorate of Idlib and town of Marea. He described the collection of information, including interviews and photographs and videos provided by interviewees and the collection of biomedical samples in the Marea investigation. While open source photographs of munitions and a black liquid were obtained, given the difficulties in accessing the area, physical evidence could not be collected for analysis. In the Idlib investigation, the FFM concluded there was likely use of a toxic chemical, probably containing the element chlorine. In the Marea investigation it was concluded with the utmost confidence that there had been exposure to sulfur mustard. The work of the FFM is on-going.

Subitem 5(c): Sampling and analysis and the role of the OPCW Laboratory and the Designated Laboratories

5.5 Dr Hugh Gregg, Head of the OPCW Laboratory, briefed participants on the OPCW Laboratory's role in off-site sample analysis and described the importance of the Designated Laboratory network. Since the United Nations investigation in 2013, the Laboratory has coordinated the analysis of almost 800 samples in support of the investigations.

Subitem 5(d): Lessons learned

5.6 Dr Ralf Trapp (an independent consultant in chemical and biological weapons arms control) briefed the workshop on the lessons learned from the Syrian missions.[15] The United Nations, the OPCW and several Member States have all undertaken lessons-learned exercises to ensure that the experiences and competences developed in these Missions will be preserved for future non-routine operations.[16,17] These discussions have focussed on strategic and operational aspects, including the political and legal requirements of such contingency operations, the management of investigations and other activities in non-permissible environments, and the development of partnerships with the different actors concerned.

5.7 Dr Trapp highlighted lessons that are relevant to enhancing the forensic capabilities of the OPCW and its network of Designated Laboratories, including the need to

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15 R. Trapp. Lessons Learned from the OPCW Mission in Syria, 2015. https://www.opcw.org/fileadmin/OPCW/PDF/Lessons_learned_from_the_OPCW_Mission_in_Syria.pdf

16 The Secretary-General's Mechanism for Investigation of Alleged Use of Chemical, Bacteriological (Biological) or Toxin Weapons: a lessons-learned exercise for the United Nations Mission in the Syrian Arab Republic; United Nations Office of Disarmament Affairs, May 2015. https://www.un.org/disarmament/publications/more/syrian-ll-report/

17 Workshop on the Lessons Learned from the International Maritime Operation to Remove and Transport the Syrian Chemical Materials in Furtherance of Security Council Resolution 2118 (2013) and Relevant OPCW Executive Council Decisions; United Nations office of Disarmament Affairs, March 2015. https://unoda-web.s3-accelerate.amazonaws.com/wp-ntent/uploads/2015/05/proceedings-maritime-public.pdf

improvise and adapt procedures to the specific circumstances at the site of investigation whilst ensuring the required level of quality assurance, scientific rigour and chain of custody. His presentation pointed out issues that require further work, including: comprehensive, accessible and curated databases; access to validated reference materials; and the need for agreed identification criteria. He also noted new opportunities emanating from advances in science and technology, such as a shift from shipping samples for off-site analysis to more sophisticated on-site analysis and transfer of data for off-site interpretation.

5.8 In the discussions of these four presentations, the following points were raised:

(a) In almost all the missions discussed, elementary chemical forensics techniques were used; they will continue to be needed to achieve the objectives of these missions, and similar missions in the future.

(b) The mandates and urgency of these missions (in particular the removal and destruction of the Syrian chemical weapons) may have resulted in some of the materials and other information potentially useful for forensic analysis being destroyed rather than archived for later review.

(c) Routine OPCW missions do not mandate collecting and archiving samples (as is routine in International Atomic Energy Agency Inspections); this can limit the availability of materials having possible future forensic analysis value.

(d) During the removal and destruction missions, handheld detection using infrared and Raman spectroscopy was employed. However, the results are indicative and have limited value for chemical forensics purposes.

(e) Approaches to integrating information from across missions were discussed, since there were overlaps of staff and mandates. In this regard, there is value in building databases that can be used to curate mission-related information for future reference and knowledge transfer (independent of whether the information is actionable at the time of curation).

(f) Training and development of investigative skill sets was recognised as critical for future work in Chemical Weapons Convention investigations. This would additionally require-thinking processes and approaches to information gathering.

(g) Non-routine investigations can involve time-critical activities; e.g. short windows of time to collect information under negotiated cease-fire situations, fluid and unpredictable security situations, etc. These investigations also involve limited (or no) on-site analysis capabilities, and collection of heterogeneous samples, such as clothing, munition fragments, etc. This can lead to incomplete data sets. Some level of flexibility may be necessary with regard to local implementation of certain details of procedures and processes.

(h) Any information that can help guide inspectors to evidence collection sites and sampling points, and what to test for, is highly valuable. Likewise, inspectors need to have access to a spectrum of capabilities to be most effective.

(i) Use of biomedical samples and the potential forensic information they might contain was also discussed. The Centers for Disease Control in the United States of America has recently shown that there are potential biomarkers for chlorine exposure.[18]

6. AGENDA ITEM SIX – Chemical Forensics and Chemical Weapons

6.1 Dr Daan Noort (TNO) moderated the session on methods for the identification of origin of chemical weapons, chemical agents and related materials.

Subitem 6(a): Identification and origin of abandoned chemical weapons

6.2 Dr Zhanshang Zhao (Ministry of National Defence, China) and Mr Cheng Tang reviewed the requirement of the Chemical Weapons Convention for abandoned chemical weapons, noting that the Technical Secretariat must retain the capability to "verify the origin of the abandoned chemical weapons and establish evidence concerning the abandonment and the identity of the Abandoning State." (Paragraph 11, Part IV (B) of the Verification Annex). They provided a case study from the abandoned chemical weapons discovered in China. The presentation discussed how the origin of an Abandoning State can easily be established in most cases through physical observation and identification; however, in some cases, it can be difficult to establish immediate scientific evidence. Examples of the latter include, abandoned chemical weapons found in bulk agent containers or those chemical agents having undergone preliminary neutralisation. Using modern analytical techniques (in particular, using $^{13}C/^{12}C$ isotopic ratios), it was possible to define the "fingerprint" of the Japanese chemical agents and to establish the Abandoning State.

6.3 In the subsequent discussion, the following point was raised:

(a) Critical to identification and tracing the origin of abandoned munitions (chemical or other) is the ability to conduct interviews, review historical records, inspect weapon design features and markings, and understand effective sampling strategies. Databases of this information should be maintained to aid future Chemical Weapons Convention related investigations.

Subitem 6(b): Position specific isotope analysis (NMR) of chemical agents

6.4 Dr Robert Williams (Los Alamos National Laboratory, the United States of America) gave a presentation entitled "Signatures for Detection and Attribution of Chemical Agents and Emerging Threats Using Site-Specific Natural Abundance Isotope Fractionation (SNIF) Nuclear Magnetic Resonance (SNIF-NMR) and Multi-Modal NMR at Ultra-Low Magnetic Fields (ULMF)". He noted that the ability to detect, identify, source, and defeat chemical threat agents is predicated on analyses that can rapidly and precisely provide forensic data about an actual or suspected use. Nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry have been used for

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[18] B. S. Crow, J. Quiñones-González, B. G. Pantazides J. W. Perez, W. R. Winkeljohn, J. W. Garton, J. D. Thomas, T. A. Blake, R. C. Johnson. Simultaneous Measurement of 3-Chlorotyrosine and 3, 5-Dichlorotyrosine in Whole Blood, Serum and Plasma by Isotope Dilution HPLC-MS-MS. *J Anal Toxicol.,* 2016; 40(4), 264-71. doi: 10.1093/jat/bkw011.
http://jat.oxfordjournals.org/content/early/2016/03/11/jat.bkw011

this purpose, but both techniques are currently difficult to employ in the field and have sample dependent sensitivity issues. Ideally, it would be optimal to have one fieldable measurement system that would be able to acquire all requisite data and perform analyses in real time to conclusively identify a suspected "unknown" threat agent, as well as provide forensic data. This "holy grail" has not yet been realised, but recent developments in SNIF-NMR and ULMF Dynamic Nuclear Polarization (DNP) enhanced J-Coupling NMR Spectroscopy (ULF-DNP-JCS) may be the next generation analytical tools that will perform the necessary functions in the field.

6.5 The presentation described efforts at Los Alamos National Laboratory to use SNIF-NMR as a quantitative tool to utilise natural abundance stable isotope ratios (e.g. $^{13}C/^{12}C$, $^{2}H/^{1}H$, etc.) at each accessible carbon or hydrogen (site-specific) in a chemical threat agent and relate the site-specific information to precursor chemicals and reagents.

6.6 Dr Williams presentation concluded with an overview of efforts to develop ULF-DNP-JCS NMR as a new, fieldable technique to identify the chemical structure of an unknown compound. J-coupling signature detection at ultra-low magnetic fields using Earth's magnetic field or a low magnetic field electromagnet is amenable for developing a portable system for the identification of Chemical Warfare Agents (CWAs), precursors, and related compounds, in non-ferrous containers.

Subitem 6(c): Chemical forensics of chemical agents

6.7 Dr Carlos Fraga (Pacific Northwest National Laboratory, United States of America) summarised research on developing a chemical forensics capability for chemical threat agents (CTAs), such as toxic industrial chemicals and CWAs. His team have used a variety of analytical and chemometric tools to demonstrate the potential of matching or excluding a CTA to a specific source (e.g. batch, precursor, manufacturer, or synthetic route). Currently, the chemical forensics of CTAs, including CWAs, is in the proof-of-concept and preliminary-assessment stages. Work to date has demonstrated the potential of using impurity profiling to link batches of sarin, cyanide salts and nitrogen mustard to their precursor chemicals.[19,20] The effects of environmental factors on a CWA simulant's impurity profile for source identification has also been initially studied. That work has shown that less volatile impurities are more persistent and likely to be better forensic signatures for source identification.[21] The potential use of stable isotope ratios to link or exclude a CWA batch to a reagent stock or another CWA sample has been recently studied. Work with commercial cyanides has provided initial evidence that products from the same

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[19] C. G. Fraga, G. A. Pérez Acosta, M. D. Crenshaw, K. Wallace, G. M. Mong, H. A Colburn. Impurity Profiling to Match a Nerve Agent to its Precursor Source for Chemical Forensics Applications. *Analytical Chemistry*, 2011, 83, 9564-9572. http://pubs.acs.org/doi/abs/10.1021/ac202340u?journalCode=ancham

[20] C. G. Fraga, K. Bronk, B. P. Dockendorff, A. Heredia-Langner. Organic Chemical Attribution Signatures for the Sourcing of a Mustard Agent and Its Starting Materials. *Analytical Chemistry*, 2016, 88, 5406-5413. http://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b00766?src=recsys

[21] C. G. Fraga, J.C. Hoggard, G. A. Pérez Acosta, L. Sego, E. Viglino, J.H. Wahl, R. E. Synovec. Preliminary Effects of Real-World Factors on the Recovery and Exploitation of Forensic Impurity Profiles of a Nerve-Agent Simulant from Office Media. *Journal of Chromatography A*, 2012, 1270, 269-282. http://www.sciencedirect.com/science/article/pii/S0021967312016640

facility/location have chemical signatures characteristic to that facility/location.[22] More work is needed to understand the fundamentals and limits of impurity profiling, stable isotope ratios and other chemical signatures for the sourcing of CTAs and/or CWAs.

6.8 In the subsequent discussion, the following points were raised:

(a) Impurity profiles and isotope ratios can be valuable for forensic analysis. Adequate training in CWA chemistry to recognise impurities at each step of a synthesis route (whether present from the beginning or formed in-process) is necessary. Suitable expertise is also required for interpretation of results.

(b) Analysis to determine the synthetic origin of chemical agents can require higher sample concentrations, which can be limiting if bulk materials are unavailable. Analysis of mixtures of CWAs and related chemicals may prove difficult.

(c) As curated archives of samples of Chemical Weapons Convention-relevant chemicals and associated data are developed, opportunities for collaboration and sharing would benefit this field of science, and OPCW's mission.

(d) Chemometrics and statistical methods are valuable in chemical forensic work.

(e) OPCW Designated Laboratories, and supporting laboratories, should seek to enhance OPCW's capacity for chemical forensics through collaborative studies (e.g. impurity profiling, and isotope ratio measurements of Chemical Weapons Convention-related chemicals). Publication of such studies is recommended to develop this scientific discipline and to strengthen the utility of Chemical Weapons Convention-related chemical forensics in the event that the data are employed as evidence in a court.

7. AGENDA ITEM SEVEN – Chemical Forensics in Law Enforcement

Subitem 7(a): On-site forensic investigations and evidence collection

7.1 Mr Cheng Tang moderated the first of two sessions looking at the experience from law enforcement, focusing on forensic investigations.

7.2 Dr Ed van Zalen (Netherlands Forensic Institute) briefed the workshop on forensics response in on-site investigations. Since 2003, the Netherlands Forensic Institute (NFI) has been developing a CBRN forensics response for the Netherlands and abroad, focusing on three pillars: (1) crime scene investigation at CBRN crime scenes; (2) traditional forensics investigation of contaminated exhibits; and (3) identification and production signatures of CBRN agents.

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[22] N. S. Mirjankar, C.G. Fraga, A.J. Carman, J. J. Moran. Source Attribution of Cyanides using Anionic Impurity Profiling, Stable Isotope Ratios, Trace Elemental Analysis and Chemometrics. *Analytical Chemistry*, 2016, 88, 1827-1834.
http://www.sciencedirect.com/science/article/pii/S0021967312016640

7.3 To conduct the examinations, the forensic scientist must ask questions such as: did an offence occur? Who committed the offence? What happened? Was the accused at the crime scene? Can dispersed materials be identified and characterised to relate them to a possible source or origin? These questions will influence the examinations conducted, the materials that are required, and/or the overall approach to the examinations by the forensic scientist, and will impact the conclusions and the final report.

7.4 Chain of custody is one of the requirements and is described as the uninterrupted control of the evidence from the crime scene to the court. Evidential material should be handled at every step if it is to be presented in court; this requires documentation showing the chronology of custody, control, transfer, receipt, or relinquishment of the items/exhibits. Also the number of individuals who handle the evidence should be limited to the smallest number possible and each transfer should be properly documented to maintain the chain of custody.

7.5 NFI is also developing innovative CBRN forensics methods, as seen in the EU Seventh Framework Programme for Research and Technological Development (FP7) where they are the coordinator for the FP7 project GIFT (Generic Integrated Forensic Toolbox to investigate CBRN incidents).[23] The procedures, equipment and methods developed in GIFT come together in the Toolbox that can be operated from a central server. A knowledge database with (open source) information is connected to the toolbox to provide the required information and procedures for the responders, crime scene investigators, laboratory scientists and the investigative authority. The toolbox is also set up to store all relevant data for a specific CBRN incident that is under investigation, meaning that all data retrieved from sensors/detectors are stored, under the chain of custody requirements for data; the outcome of all laboratory investigations are stored; 3D images and the registration of the crime are stored; and the registration and authentication data of all secured and seized exhibits are stored. GIFT will enable the investigative authority and forensic investigators to have direct online access to all incident-related information that they might need for their work. The methods, equipment and procedures developed within GIFT will meet the requirements for accreditation by ISO17020 for crime scene investigation and ISO17025 for laboratory investigations.

7.6 Mr Jari Pukkila (National Bureau of Investigation Forensic Laboratory, Finland) described the general principles of crime scene operations, evidence collection and sample handling. He emphasised that inter-agency cooperation can allow forensics to be applied to evidence collected outside the direct control of a given forensic laboratory (this is important as different agencies respond to different kinds of incidents, yet have capabilities that are beneficial to one another). He further noted that authority co-operation is the cornerstone in preparedness to CBRNE incidents. He provided a view of quality control across the whole chain of forensic operations from scene investigations to court reporting, and described how procedures are harmonised on a European level.

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[23] See www.giftforensics.eu

7.7 In the subsequent discussion, the following points were raised.

(a) Everything leaves a trace in the chain of custody and handling of evidence. It is important to minimise handling/processing and to understand its impact.

(b) Informatics tools (e.g. radiofrequency identification (RFID) tags and scanners, fieldable sensors, smart devices, etc.) can help ensure chain of custody, and allow processing and archiving of information at the point of evidence collection. The OPCW may benefit from the applicability of such tools to its operations.

(c) The GIFT project may be informative for the development of on-site data collection software useful to OPCW missions.

(d) It is important to document as thoroughly as possible, the history of a chemical incident, to select optimal sampling points, and run simulation experiments to support conclusions.

Subitem 7(b): Forensic chemistry, forensic intelligence and illicit drugs

7.8 Professor Slawomir Neffe moderated the second session on law enforcement experience, looking at examples of illegal drug attribution.

7.9 Professor Claude Roux and Dr Marie Moreleto (Centre for Forensic Science, University of Technology, Sydney, Australia) briefed the workshop on challenges and opportunities of forensic intelligence relevant to the Chemical Weapons Convention, asking the question: "can we learn from the illicit drug profiling experience?". The presentation provided an overview of forensic intelligence and the role it plays in forensic science through its extension of the forensic case-by-case approach (i.e., evidential focus) into a more phenomenological and proactive approach.[24] Forensic intelligence focuses on the criminal activity. Its role is not solely limited to investigations or to confirm hypotheses suggested by conventional police means, but also to proactively provide insights into criminal activity and to support the elicitation of relevant hypotheses.[25] The development of forensic intelligence relies on the expression of suitable models that assist in comparing and evaluating methods and new technologies, providing transparency and fostering the development of new applications.[26]

7.10 Illicit drug profiling was used as an example. Illicit drug analysis can serve different purposes in the forensic process. Its primary use is to investigate a particular case

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[24] O. Ribaux. *Police Scientifique, le Renseignement par la Trace*, Presses Polytechniques et Universitaires Romandes, Lausanne, 2014.

[25] M. Morelato, S. Baechler, O. Ribaux, A. Beavis, M. Tahtouh, P. Kirkbride, C. Roux, P. Margot. Forensic Intelligence Framework - Part I: Induction of a Transversal Model by Comparing Illicit Drugs and False Identity Documents Monitoring. *Forensic Science International* 2014, 236, 181-190. http://www.fsijournal.org/article/S0379-0738(14)00016-4/abstract

[26] S. Baechler, M. Morelato, O. Ribaux, A. Beavis, M. Tahtouh, K. P. Kirkbride, P. Esseiva, P. Margot, C. Roux. Forensic Intelligence Framework. Part II: Study of the Main Generic Building Blocks and Challenges Through the Examples of Illicit Drugs and False Identity Documents Monitoring. *Forensic Science International*, 2015, 250, 44-52. http://www.fsijournal.org/article/S0379-0738(15)00087-0/abstract

(i.e. illicit drug identification and purity determination for court purposes). Its secondary use is to infer series of crime (i.e. link seizures through physical or chemical profiles and supportive action of law enforcement agencies). Its tertiary use is to provide knowledge about crime phenomena and illicit drug networks (i.e. level of distribution, trends, estimation of the consumption through waste water analysis).

7.11 Using Australian Federal Police (AFP) case data, in particular different chemical profiles of 3,4-methylenedioxymethylamphetamine (MDMA), a statistical procedure was developed to compare illicit drug profiles. This procedure was performed using a specific comparison metric previously chosen and optimised. The degree of relationship between the profiles was returned as a score, providing the closeness between two profiles. A binary classification was used to determine the existence of a link between specimens. A link was thus either existent or non-existent according to a threshold value previously determined using a reference population. It was demonstrated that chemical profiling of illicit drugs can be used to go beyond simply refuting or confirming a connection between cases. The current AFP chemical profiling approach applied to MDMA specimens involves numerous analytical techniques, but it was shown that the use of only one profiling technique was adequate to obtain more timely intelligence products that could be used in an operational intelligence perspective.[27] Finally, a general and multi-commodity model was proposed. It is believed that this model could guide the use of any forensic case data. It is further hypothesised that the model could be applied to chemical warfare data in an intelligence-led perspective.

7.12 Dr Veronica Borrett gave a presentation provided by Dr Michael Collins (Director of the Australian Forensic Drug Laboratory, National Measurement Institute (NMI), Sydney Australia). The presentation provided an overview of the illicit drug profiling programme that NMI undertakes for the AFP. The programme includes determination of the geographic origin of cultivated and semi-cultivated drugs, such as cocaine and heroin, and the synthetic route used to produce drugs such as methylamphetamine. The presentation outlined the main drug signatures of which stable isotope ratio analysis is one, and gave a brief outline of profiling approaches including alkaloid analysis, solvent profiles, diluents and additives, which can provide profile information and that can complement the isotope signatures.

7.13 The presentation focused on methylamphetamine as it best illustrates the use of the isotope signature and, as a fully synthetic drug, may provide parallels for the development of analytical procedures for samples relevant to the Chemical Weapons Convention. Methylamphetamine is prepared from ephedrine or pseudoephedrine, two pharmaceuticals that may be produced industrially by three major routes: (1) extraction on a large scale from the Ephedra species; (2) semi-synthetic from a sugar source and benzaldehyde; and (3) fully synthetic from phenyl-2-propanone. The ephedrine made by these three routes has three distinct isotope ratio profiles. These profiles are carried through to the final product methylamphetamine. By determining the C, H and N stable isotope ratios in methylamphetamine it is possible to determine the type of precursor chemical that was used.

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[27] M. Morelato, A. Beavis, M. Tahtouh, O. Ribaux, K. P. Kirkbride, C. Roux. The Use of Organic and Inorganic Impurities Found in MDMA Police Seizures in a Drug Intelligence Perspective. *Science & Justice*, 2014, 54, 32-41. http://www.scienceandjusticejournal.com/article/S1355-0306(13)00084-1/abstract

7.14 In the subsequent discussion, the following points were raised:

(a) The integration of analytical chemistry with unstructured data sets (observations and annotated meta-data) can be a powerful tool for discovering actionable information. The methods developed in law enforcement for chemical samples are valuable. Training inspectors in these approaches would strengthen the capabilities of the Secretariat for contingency operations.

(b) Producing data sets and indicators for recognition of certain characteristics (or sources of origin) of chemical agents, such as those produced in law enforcement for illicit drug attribution, would be beneficial for Chemical Weapons Convention verification-related activities. How to overcome challenges in building adequate data sets that can be applied over broad parameter space will need to be considered.

(c) The utility of stable isotope ratio analysis for drug profiling was noted. Its application to the analysis of samples containing Chemical Weapons Convention-relevant chemicals should be studied further.

8. AGENDA ITEM EIGHT – Biomedical Samples

8.1 Professor Slavica Vučinić (National Poison Control Centre, Military Medical Academy, Serbia) moderated a session on biomedical sample analysis, covering forensic and chemical weapon investigation-related toxicology perspectives.

Subitem 8(a): Forensic toxicology

8.2 Dr Anna Pelander (Forensic Toxicology Unit, National Institute for Health and Welfare, Finland) briefed the workshop on the key role that forensic toxicology plays in cause-of-death investigations. According to Finnish legislation, forensic toxicological investigation is requested by the pathologist performing the autopsy, or the police. The most important sample matrices for forensic toxicological investigation are whole blood and urine. Liver, vitreous humour, stomach contents, muscle, bile, and hair may also be analysed. Analysis of alternative matrices is often unavailable, for example due to decomposition. Target analytes include alcohols, other volatile chemicals, therapeutic and illicit drugs, natural poisons, pesticides, etc. The wide scope causes a continuous challenge for the techniques applied. During the last decade the surge of new psychoactive substances (NPS) has raised the challenge to a higher level. However, the emergence of tandem and high resolution mass spectrometry, with wide-scope applications, has enabled the laboratories to cope with the constantly expanding number of substances with potential for abuse.

8.3 In the subsequent discussion, the following points were raised:

(a) NPS are challenging due to their constant appearance, huge chemical diversity, frequent changes of composition of preparations, and difficulties in identification and characterisation.

(b) Whole blood samples are the most important samples in post-mortem analysis as reference data are available (noting that reference data measured in serum or plasma will vary from whole blood).

(c) Retrospective information about drug usage can in some cases be obtained from hair samples. Some participants mentioned problems they had experienced with the utility of hair samples; however, it was also noted that there have been publications on the use of hair or keratin samples for detecting chemical agent exposure.[28, 29, 30]

(d) The NFI mass spectral database contains accurate masses of substances and metabolites and can be used in lieu of reference standards in some cases. Conclusive results, however, do require comparison to reference standards.

Subitem 8(b): Biomedical samples in chemical weapons and toxins analysis

8.4 Mr Martin Söderström (Laboratory Coordinator of VERIFIN, University of Helsinki, Finland) provided a presentation entitled "Biomedical samples in chemical weapons analysis". He gave an overview on the actions of chemical warfare agents on humans and the ways exposure to these agents can be detected. Several characteristic chemical warfare agent metabolites can be found in biomedical samples. The duration from the exposure to sampling will determine which metabolites can be detected. Adducts with biomolecules in blood can be detected up to one month after exposure. It may be difficult to determine the absolute dose the person was exposed to, but the effects on the patient can be seen, e.g. in the ratios of adducted and native biomolecules in the sample. During an investigation of alleged use, both environmental and biomedical samples need to be taken, as they have different functions: environmental samples are used prove the identity and possibly the origin of the agent, while biomedical samples show the extent of exposure of people in the area. The main sample types for biomedical samples are blood and urine, but depending on the case, additional samples, such as hair and tissue samples, could be taken. If sampling is not witnessed by the investigation team, the samples should be matched with the patient using DNA analysis.

8.5 Dr. Rudolph Johnson (Chief of the Emergency Response Branch at the Division of Laboratory Sciences, National Center for Environmental Health, US Centers for Disease Control and Prevention (CDC)) provided a presentation entitled "Measuring Human Exposure to Nerve Agents and Marine Toxins". He reviewed determinations of organophosphorus nerve agent metabolites and protein adducts in urine, blood and blood spots. He demonstrated that high confidence determinations can be achieved through a combination of isotope dilution liquid chromatography-tandem mass spectrometry (LC/MS/MS) and butyrylcholinesterase activity techniques in urine, blood or blood spots. Commonly tested biomarkers of nerve agent exposure included hydrolysis products or protein adducts to butyrylcholinesterase or albumin. A short

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28 M. Spiandore, A. Piram, A. Lacoste, D. Josse, P. Doumenq. Hair Analysis as a Useful Procedure for Detection of Vapour Exposure to Chemical Warfare Agents: Simulation of Sulphur Mustard with Methyl Salicylate. *Drug Test Analysis*, 2014, 6, 67–73. doi: 10.1002/dta.1659. http://onlinelibrary.wiley.com/doi/10.1002/dta.1659/abstract

29 A.S. Appel, J. H. McDonough, J. D. McMonagle, B. A. Logue. Analysis of Nerve Agent Metabolites from Hair for Long-Term Verification of Nerve Agent Exposure. *Anal. Chem.*, 2016, 88 (12), 6523 -6530.DOI: 10.1021/acs.analchem.6b01274. http://pubs.acs.org/doi/abs/10.1021/acs.analchem.6b01274

30 J. L. S. Sporty, S. W. Lemire, E. M. Jakubowski, J. A. Renner, R. A. Evans, R. F. Williams, J. G. Schmidt, M. J. van der Schans, D. Noort, R. C. Johnson. Immunomagnetic Separation and Quantification of Butyrylcholinesterase Nerve Agent Adducts in Human Serum. *Anal. Chem.*, 2010, 82, 6593-6600. http://pubs.acs.org/doi/abs/10.1021/ac101024z

review of saxitoxin, gonyautoxins, or tetrodotoxin exposure testing was also presented using offline and online solid phase extraction and LC/MS/MS.

8.6 The Rapid Toxic Screen (RTS), a comprehensive laboratory testing protocol at the CDC, was also reviewed. The RTS is used following an unknown chemical exposure from vesicants, toxic metals, cholinesterase inhibitors, cyanide, volatile organic compounds, rodenticides, or other new agents. Exposure to these chemical agents is measured in the first 40 highly exposed individuals, within 36 hours of delivery to the CDC.

8.7 Professor Paula Vanninen reviewed the aims of the European Union-funded TOXI-triage project "Integrated and Adaptive Responses to Toxic Emergencies for Rapid Triage: Engineering the Roadmap from Casualty to Patient to Survivor".[31] In this four-year project there are 18 partners and nine work packages. The project has seven principal objectives: accelerated delivery of situational awareness; command and control with secure, dynamic, and seamless communication; traceable point-of-care diagnostic tests with integrated casualty tracking; comprehensive field toolbox for CBRN threats for end users; protocol for the registration of biomarkers of injury from CBRN poisoning; establish a harmonised European framework for ethical and accountable civilian CBRN operations; establish a community of commerce; and deliver a commercial vision. Within this project, emerging technologies are also being explored; these include non-invasive breath analysis, remote piloted airborne systems, hyperspectral imaging, and aptamers. Results of the project will be available in 2019.

8.8 In the subsequent discussion, the following points were raised:

(a) Biomedical samples from casualties of chemical warfare agent exposure are rare and should be exploited forensically as much as possible, to obtain to the maximum amount of information.

(b) Some metabolites are not unique: they may not be conclusive for exposure, but may provide supporting information to an investigation.

(c) Reference samples are needed, however, not all metabolites can be reproduced with spiking. Archives of patient samples are extremely valuable.

(d) Understanding the impact of collection equipment, e.g. additives in tubes, is extremely important in interpreting results.

(e) The anticoagulant used in blood sample collection needs to be stated to the laboratory undertaking the analysis. Blood cells and plasma should be separated from the blood samples as soon as possible, as storing whole blood in a freezer leads to cell breakage.

(f) Blood spot analysis papers are useful for analytical purposes, but shipping can be problematic due to transport regulations.

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[31] See http://www.toxi-triage.eu/

(g) Poisoning by chemicals may have different characteristics than those caused by a CBRN weapon (toxins in food for example). It would be of value to understand how these cases have been identified. Such work would provide examples of forensic methods and approaches that may be relevant to Chemical Weapons Convention-related chemical analysis.

(h) Chemical warfare agent tests have not been standardised (no commercial need at this point). Credibility relies on proficiency testing and publications.

(i) Sufficient sample amount can be an issue when samples are subjected to multiple methods.

9. AGENDA ITEM NINE – Other Attribution Analysis

9.1 Professor David Gonzalez moderated a session on attribution analysis used in food safety and art.

Subitem 9(a): Food safety and toxins

9.2 Dr Jacques-Antoine Hennekinne (French Agency for Food, Environmental and Occupational Health and Safety) briefed the workshop on managing and characterising staphylococcal food poisoning outbreaks from the food vehicle to the incriminated source. Staphylococcal food poisoning is one of the most common food-borne diseases and results from the ingestion of staphylococcal enterotoxins (SEs) preformed in food by enterotoxigenic strains of coagulase positive staphylococci mainly *Staphylococcus aureus*. To date, more than 20 SEs have been described. All SEs have superantigenic activity whereas only a few have been proved to be emetic, representing a potential hazard for consumers. Characterisation of staphylococcal food poisoning outbreaks (SFPOs) has progressed considerably compared to 50 years ago, when staphylococci were simply enumerated and only five enterotoxins were known for qualitative detection. Today, SFPOs can be characterised by a tool box including the identification of *S. aureus* biovars, the use of molecular based-methods to identify pathogenic factors, the specific immunodetection for SEs, and the absolute quantification by mass spectrometry based-methods.[32] After an introduction focusing on the food poisoning reporting scheme and the associated data at the European Union level,[33] Dr Hennekinne's presentation provided examples focused on the need to characterise such events properly, using examples of integrated bacteria-to-protein approaches for characterising staphylococcal food poisoning events.

9.3 In the subsequent discussion, the following point was raised:

(a) Availability of reference materials is critical to avoid misinterpretation of food poisoning events, to assist emergency responders and decision makers.

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[32] J.-A. Hennekinne, M.-L. De Buyser, S. Dragacci. *Staphylococcus aureus* and its Food Poisoning Toxins: Characterization and Outbreak Investigation. *FEMS Microbiology Reviews*, 2012, 36, 815–836. http://onlinelibrary.wiley.com/doi/10.1111/j.1574-6976.2011.00311.x/full

[33] The European Union Summary Report on Trends and Sources of Zoonoses, Zoonotic Agents and Food-borne Outbreaks in 2014. *EFSA Journal*, 2015, 13, 4329. doi: 10.2903/j.efsa.2015.4329. https://www.efsa.europa.eu/en/efsajournal/pub/4329

Subitem 9(b): Chemical forensics and art

9.4 Professor Juhani Huuskonen (University of Jyväskylä and RECENART® Inc., Finland) briefed the workshop on the use of chemical forensics in art - a field where a large percentage of the objects sold are either forgeries or copies - with a connoisseur-tradition where authentication of the art piece is done by visual inspection by an individual with a trained "eye" and special knowledge of certain artists. Current research and analysis in the field is based on a combination of materials science and historical research; providing more accurate outcomes than connoisseur statements. In the art world, attribution means the authorship of a work of art. To determine the attribution it is necessary to study style, subject, provenance, technique and materials. Together this helps contextualise the work of art. Material analysis (of pigments and other materials) gives an estimation of the age of an art piece, and can also reveal a forgery. X-Ray Fluorescence (XRF), Raman, Fourier-Transform-Infrared (FT-IR), light microscopy, polarised-light microscopy, chromatography and imaging methods are commonly used for pigment and material analysis.

9.5 In the subsequent discussion, the following points were raised:

(a) Handheld screening instruments are used at "point of care" in artwork analysis. Hyperspectral imaging in the visible and near-infrared modes is often used to generate a spectrum for individual segments of a painting. Likewise, destructive sampling of expensive artwork is performed using micro-samples to minimise any detrimental impact.

(b) The existence of many natural and synthetic dyes creates a large number of possible chemical signatures that need to be considered when performing art authentication analysis. Conceptually, this produces similar challenges to forensic analysis of drugs of abuse.

10. AGENDA ITEM TEN – Reconstructing Past Events

10.1 Professor Ramasami Ponnadurai moderated the final technical session looking at chemical forensics in archaeology.

Subitem 10(a): Chemical forensics in archaeology

10.2 Professor Richard Evershed (University of Bristol, United Kingdom of Great Britain and Northern Ireland) described how archaeologists combine biomolecular and isotopic techniques to probe human prehistory. He described how the technological advances of recent years have had a major impact on all areas of archaeology making it possible to answer hitherto intractable questions concerning the activities of our ancestors. One area where progress has been particularly rapid is the application of analytical chemistry in investigation of organic residues preserved at a wide variety of locations at archaeological sites, such as human remains, pottery vessels, soils, plant remains, etc. The analytical chemical challenge is that such materials are by their very nature complex mixtures of biochemical components, made still more complex by decay and human activity. However, such is the power of modern analytical chemistry that we can now address such questions as: What plants and animals did

ancient peoples eat? How did they treat their dead? What did they use for fertiliser? What organic natural products did they use for glues, lubricants and lighting?

10.3 Professor Evershed noted that answering such questions requires interrogation of the preserved biomolecular components of residues using chromatographic and mass spectrometric (MS) techniques to separate and identify molecular structures that can be matched to those of biochemical components found in modern living organisms, likely to have been exploited by humans in the past. This biomarker approach[34] is enhanced by instrumental developments in isotope ratio MS and accelerator MS allowing compound-specific isotope compositions to be recorded for a range of elements common to major biochemical components of animals and plants (C, H, N, etc.). This linking of molecular structure-to-isotopic composition increases the diagnostic value of commonly occurring preserved biomarkers, such as lipids and proteins, allowing exploitation of previously inaccessible information relating to metabolism, digestive physiology, environment, climate and absolute age, thereby enhancing provenance assignments. This approach has found applications beyond archaeology in criminal[35] and food[36] forensics.

10.4 Professor Patrick Degryse (Centre for Archaeological Sciences at the Katholieke Universiteit Leuven, Belgium) provided a presentation on provenance, technology, exchange and trade of inorganic materials in an archaeological context by examining isotopic evidence. The study of the history and technology of ancient materials has always been an essential part of archaeological and anthropological research; especially the origin of raw materials, their transformation into objects and their exchange/trade have been topics of investigation. As soon as chemical techniques were introduced to archaeological research, the use of isotopic analysis was explored. Methodologies were often borrowed from geochemistry, possibly adapted to archaeological-anthropological research questions. Early use of isotopic analysis in archaeological science included oxygen and carbon isotopes for marble provenancing and lead isotopic work to determine the origin of copper alloys and glass. The nature of archaeological research and the sometimes unpredictable aspects of human behaviour necessitates careful interpretation of geochemical data; this is not always straightforward.

10.5 The past decade has seen an increase in the number of isotopic studies for archaeological and forensic purposes. Importantly, the use of isotopic systems particularly developed to answer specific archaeological or forensic questions, has become more frequent. Examples are the use of strontium to study human mobility and vitreous materials, neodymium and boron to study glass, and copper and antimony to study the early development of pyrotechnology in vitreous materials and

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34 R. P. Evershed. Organic Residue Analysis in Archaeology: The Archaeological Biomarker Revolution. *Archaeometry*, 2008, 50, 895-924. http://onlinelibrary.wiley.com/doi/10.1111/j.1475-4754.2008.00446.x/abstract

35 I. D. Bull, R. Berstan, A. Vaas. R. P. Evershed. Identifiaction of a Disinterred Grave by Molecular and Stable Isotope Analysis. *Science & Justice*, 2009, 49, 142-149. http://www.ncbi.nlm.nih.gov/pubmed/19606594

36 H. Mottram, S. E. Woodbury, J. B. Rossell, R. P. Evershed. High-resolution detection of adulteration of maize oil using multi-component compound-specific $\delta^{13}C$ values of major and minor components and discriminant analysis. *Rapid Commun. Mass Spectrom*, 2003, 17, 706-712. http://onlinelibrary.wiley.com/doi/10.1002/rcm.947/abstract

metals. The origins of materials, the provenance of the raw materials used in their making, and the mobility of humans are crucial aspects in the study of the history of exchange, trade and ancient society. However, it is has become more and more clear that correct interpretation of geochemical data, and a translation to an archaeological-anthropological-forensic reality, is necessary. Custom-made isotopic procedures, answering questions related to chemical weapons ingredients or their provenance may therefore have potential, similar to the development and use of these techniques in archaeology. Professor Degryse provided the workshop with some representative technical papers on these methods for further review.[37,38,39,40]

10.6 In the subsequent discussion, the following points were raised:

(a) Archaeological databases may contain isotopic ratios for materials originating from specific geolocations, information that might be helpful in forensic analysis of certain types of samples (or other evidence with environmental signatures).

(b) Soil science databases and sample archives may also provide important reference materials useful to Chemical Weapons Convention investigations.

(c) The principles governing the survival of organic compounds in archeology have many similarities with those relating to the survival of chemical warfare agents in environmental material, e.g. adsorption or encapsulation.

(d) Impurity profiles are routinely used in archaeology, especially for provenancing raw materials used in the production of cultural objects.

(e) Inorganic impurities (possibly from production equipment) may be of relevance, for example, boron and strontium isotopes from glass. The materials used in munitions (shell casings and energetic materials) also have characteristic inorganic signatures. Portable X-ray fluorescence systems, such as those used in art analysis, can quickly provide information on inorganic components.

(f) Similar to art analysis, microscale sampling has been extensively developed for archaeological samples.

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37 P. Degryse (Ed.). *Glass Making in the Greco-Roman World*, Leuven: Leuven University Press, 2014.

38 P. Degryse, J. Schneider. Pliny the Elder and Sr-Nd Isotopes: Tracing the Provenance of Raw Materials for Roman Glass Production. *Journal of Archaeological Science*, 2008. 35, 1993-2000. http://www.sciencedirect.com/science/article/pii/S0305440308000083

39 P. Degryse, L. Lobo, A. Shortand, F. Vanhaecke, A. Blomme, J. Painter, D. Gimeno, K. Eremin, J. Greene, S. Kirk, M. Walton. Isotopic Investigation into the Raw Materials of Late Bronze Age Glass Making. *Journal of Archaeological Science*, 2015, 62, 153-160. http://www.sciencedirect.com/science/article/pii/S0305440315002411

40 V. Devulder, F. Vanhaecke, A. Shortland, D. Mattingly, C. Jackson, P. Degryse. Boron Isotopic Composition as a Provenance Indicator for the Flux Raw Material in Roman Natron Glass. *Journal of Archaeological Science*, 2014, 46, 107-113. http://www.sciencedirect.com/science/article/pii/S0305440314000880

11. AGENDA ITEM ELEVEN – Breakout Groups

11.1 Workshop participants were divided into four breakout groups to address key questions related to chemical forensics for chemical weapons investigation purposes.

11.2 The first breakout group facilitated by Dr Veronica Borrett addressed the question "How can chemical forensics be combined with investigative chemical analysis?". In the discussion, the following points were raised:

(a) The establishment of a temporary working group on the development and application of forensic methodologies, to support OPCW inspectors within the mandate of the OPCW, could be valuable to allow further consideration of how to use these methods for Chemical Weapons Convention implementation. Topics of consideration could include the development of forensic methods for crime investigation and traditional forensics methods and procedures within the OPCW's mandate. Forensic approaches could help to connect materials, persons and events to any intentional criminal or terrorist activity.

(b) Determine the best approach for supporting the OPCW's inspectors to enhance forensic awareness and forensic investigation capabilities. This may include additional forensic training and/or reachback capabilities to scientific expertise.

(c) Laboratories could review and augment their procedures regarding future forensic exploitation and retention of stored samples acquired during investigations.

(d) The SAB and/or the Secretariat might review the potential of impurity profiling, in particular inorganic profiles, in relation to extraction of forensic information to support investigations of alleged use.

(e) Consideration could be given to establishing a system for the management of data, including the collection, curation and mining of data. To do this, support is needed to define the requirements and the associated support infrastructure.

(f) A review of past studies - e.g. OPCW SAB studies - and partner information could be valuable for updating and refining Recommended Operating Procedures for collecting and analysing biomedical samples. This could provide useful advice on samples types, their collection, preservation and transportation.

(g) Autonomous systems have value in supporting investigations of alleged use of chemical weapons. Reviewing how these systems could be used in the broader investigative picture, as well as for sampling and on-site analysis/detection systems, would be informative.

(h) In regard to data and evidence collection, internet available information in a simplified form on how to best take and preserve samples in an investigation of alleged use would be beneficial for on-site investigators.

11.3 The second breakout group facilitated by Professor Volodymyr Zaitsev addressed the question "Limitations and required reference materials?". In the discussion, the following points were raised:

(a) The group emphasised the forensic and analytical value of authentic samples and associated meta data. This could include scheduled chemicals, derivatives, precursors, degradation products, and other samples of forensic relevance.

(b) The group suggested identifying the availability of Chemical Weapons Convention-relevant archived materials. A first step could be a survey of the Designated Laboratories.

(c) Importance was placed on engaging with a broader network, for example law enforcement, regulatory, food safety, agricultural, archeological, public health and environmental testing organisations.

11.4 The third breakout group facilitated by Dr Robert Mikulak addressed the question "Methodologies with potential for use in CW applications?". In the discussion, the following points were raised:

(a) The group considered that chemical forensic methods can play an important role in verification of the Chemical Weapons Convention, but noted that forensic information is seldom definitive and must be integrated with other available information.

(b) The group noted the demonstrated forensic value of environmental and biomedical samples for determining whether or not chemical weapons have been used. It noted the recent development of biomedical sampling methods for determining exposure to chlorine and suggested that consideration be given to the development of biomedical methods for determining exposure to some other toxic industrial chemicals that might be used as chemical weapons.

(c) The group recognised the value of further exploration and development of methods using impurity profiling and isotopic ratio determination for attribution purposes, for example: related to determining responsibility for use of chemical weapons, for abandoned chemical weapons, or for clandestine chemical weapons production. The possible use of impurities not related to the product, such as solvents or inorganic elements, should also be considered.

(d) The group recognised a need for a database for forensic purposes that could include existing analytical data on abandoned chemical weapons and on impurity profiles for known synthetic routes to chemical warfare agents.

(e) The group recognised the need for management software for data collected during field investigations, including forensic data. In this connection, it noted the sophisticated software being developed as part of the GIFT project, as briefed during the workshop.

(f) The group would like to see the SAB explore further the use of chemical forensics in Chemical Weapons Convention verification, possibly through a temporary working group and with the assistance of forensic experts.

11.5 The fourth breakout group facilitated by Mr Valentin Rubaylo addressed the question "Normal samples vs. highly toxic samples?". In the discussion, the following point was raised.

(a) It is important to develop capabilities for the sampling and analysis of samples from incidents involving toxic industrial chemicals that are not included in the Annex on Chemicals of the Convention.

12. AGENDA ITEM TWELVE – Adoption of the Report

The SAB and other participants considered and adopted the report of the workshop on "Chemical Forensics: Capabilities across the Field and the Potential Applications in Chemical Weapons Convention Implementation".

13. AGENDA ITEM THIRTEEN – Closure of the Workshop

The Chairperson closed the workshop at 15:35 on 22 June 2016.

Annex: List of participants in workshop on "Chemical Forensics: Capabilities across the Field and the Potential Applications in Chemical Weapons Convention Implementation"

Annex

LIST OF PARTICIPANTS AT THE WORKSHOP ON "CHEMICAL FORENSICS: CAPABILITIES ACROSS THE FIELD AND THE POTENTIAL APPLICATIONS IN CHEMICAL WEAPONS CONVENTION IMPLEMENTATION"

	Participant	Institution
1.	Mr Dominique Anelli	Consultant, France
2.	Dr Augustin Baulig*	Secrétariat général de la défense et de la sécurité nationale, Paris, France
3.	Dr Gaëtan Benac-Lestrille	DGA Maitrise NRBC, France
4.	Dr Veronica Borrett*	BAI Scientific and Honorary Fellow University of Melbourne, Australia
5.	Dr Christophe Curty*	Spiez Laboratory, Switzerland
6.	Professor Patrick Degryse	Centre for Archaeological Sciences at the Katholieke Universiteit Leuven, Belgium
7.	Professor Richard Evershed	University of Bristol, United Kingdom of Great Britain and Northern Ireland
8.	Dr Jonathan Forman	Organisation for the Prohibition of Chemical Weapons, The Hague, the Netherlands
9.	Dr Carlos Fraga	Pacific Northwest National Laboratory, Richland, Washington, United States of America
10.	Dr David Gonzalez*	Department of Chemistry, University of the Republic of Uruguay, Montevideo, Uruguay
11.	Dr Hugh Gregg	Organisation for the Prohibition of Chemical Weapons, The Hague, the Netherlands
12.	Dr Kirsi Harju	VERIFIN, Finland
13.	Dr Jacques-Antoine Hennekinne	French Agency for Food, Environmental and Occupational Health and Safety (Anses)
14.	Professor Juhani Huuskonen	University of Jyväskylä and RECENART® Inc., Finland
15.	Dr Rudolph Johnson	Emergency Response Branch at the Division of Laboratory Sciences, National Center for Environmental Health, US Centers for Disease Control and Prevention, United States of America
16.	Dr Karoliina Joursiniemi	VERIFIN, Finland
17.	Ms Maaret Karjalainen	VERIFIN, Finland
18.	Mr Harri Kiljunen	VERIFIN, Finland
19.	Mr Tatu Köli	VERIFIN, Finland
20.	Dr Harri Koskela	VERIFIN, Finland
21.	Ms Marja-Leena Kuitunen	VERIFIN, Finland
22.	Mr Matti Kuula	VERIFIN, Finland
23.	Ms Astrid Lewis	United States Department of State
24.	Professor Roberto Martinez-Alvarez*	Complutense University, Madrid, Spain
25.	Dr Robert Mikulak*	United States Department of State (retired)

	Participant	Institution
26.	Dr Marie Morelato	Centre for Forensic Science, University of Technology Sydney, Australia
27.	Professor Slawomir Neffe*	Military University of Technology, Warsaw, Poland
28.	Ms Hanna Niemikoski	VERIFIN, Finland
29.	Dr Daan Noort	Netherlands Organisation for Applied Scientific Research (TNO)
30.	Ms Irene O'Sullivan	Netherlands Forensic Institute, The Hague, the Netherlands
31.	Dr Simon Ovenden	DSTO Group, Australia
32.	Ms Marlene Payva	Organisation for the Prohibition of Chemical Weapons, The Hague, the Netherlands
33.	Dr Anna Pelander	National Institute for Health and Welfare, Forensic Toxicology, Helsinki, Finland
34.	Ms Annette Pettersson	VERIFIN, Finland
35.	Mr Lennie Phillips	Organisation for the Prohibition of Chemical Weapons, The Hague, the Netherlands
36.	Mr Jari Pukkila	National Bureau of Investigation (NBI) Forensic Laboratory, Finland
37.	Professor Ponnadurai Ramasami*	University of Mauritius
38.	Ms Marja-Leena Rapinoja	VERIFIN, Finland
39.	Dr Syed K. Raza*	Institute of Pesticide Formulation Technology (IPFT), India
40.	Dr James Riches	Defence Science and Technology Laboratory (Dstl), Porton Down, United Kingdom of Great Britain and Northern Ireland
41.	Professor Claude Roux	Centre for Forensic Science, University of Technology Sydney, Australia
42.	Mr Valentin Rubaylo*	State Scientific Research Institute of Organic Chemistry and Technology, Russian Federation
43.	Dr Susanna Salminen-Paatero	University of Helsinki, Finland
44.	Ms Kira Sivula	VERIFIN, Finland
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