OPCW Technical Secretariat

S/2214/2023
9 October 2023
ENGLISH only

NOTE BY THE TECHNICAL SECRETARIAT

REPORT OF THE FIFTY-SIXTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 13 – 14 SEPTEMBER 2023

1. The Validation Group met on 13 and 14 September 2023 to discuss the evaluation of analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD) and to consider matters related to this database. Mr Brian Mayer (United States of America) served as the Chairperson of the meeting. The meeting was held in a hybrid format, with some members attending in person and others joining via video conference. Meetings addressing data review were held in accordance with the subgroup coordinators' preferences.

2. The evaluators for the analytical techniques evaluated new data and reported to the coordinators for each analytical technique. The names of the coordinators who were present at the meeting, along with the technique for which each was responsible, are listed below.

Mr Gary Mallard (United States of America)	Gas chromatography (retention index) (GC(RI))
Ms Karin Höjer Holmgren (Sweden)	Mass spectrometry (MS)
Mr Armando Alcaraz (United States of America)	Infrared (IR) spectroscopy
Mr Damian Magiera (Germany)	Nuclear magnetic resonance (NMR) spectroscopy

3. Mr Harri Heikkinen (Finland) announced his resignation from the Validation Group. The Group thanked him for his contributions, and wished him well in his next assignment.

4. The coordinators provided an evaluation summary of the data submitted to the Validation Group for discussion at the meeting. The evaluators finalised their evaluation of the analytical data and confirmed that the approved data was technically valid.

5. The Validation Group discussed several matters relating to data submission and evaluation. First, members agreed to stop using the "C" designation for unaccepted data and to use only "N" since the two designations are procedurally equivalent: "C" will no longer be used as an evaluation designation. The definition of "P" (namely, "postponed") was clarified by members to mean simply "no decision was made". This designation may be used in the event that there is a lack of agreement among subgroup members, or when there is an insufficient number of available evaluators.

6. The Validation Group recommended that submission laboratories now provide a Simplified Molecular Input Line Entry Specification (SMILES) notation along with their data for review. Additionally, the OPCW Laboratory will begin adding SMILES notations to approved data in the OCAD and the Validation Group Working Database.

7. The Validation Group discussed how to encourage laboratories to submit data for chemicals listed in Schedules 1.A.13, 1.A.14, 1.A.15, and 1.A.16. The Group acknowledged that submission laboratories might be reluctant to provide data, so the Group discussed the practicalities of anonymising submissions (if requested) prior to Group review. The Group also recommended the OPCW Laboratory to provide laboratories with prioritisation to better guide synthesis and data acquisition efforts. The Group also recommended that all laboratories— not just designated laboratories— be encouraged to submit data to the OCAD and the Validation Group Working Database.

8. The Validation Group discussed the possibility of including data associated with biomedical signatures (such as protein adducts) and biotoxins (such as saxitoxin and ricin). The Group also discussed considering synthetic opioids (fentanyl-based compounds, for example). The Group agreed to discuss interest in this endeavour with their home organisations and will continue the conversation when the Group reconvenes in spring 2024.

9. The Group discussed how to increase participation in the Validation Group. The Group recommended that the OPCW Laboratory continue to remind proficiency test meeting participants that any scientific staff can be nominated for Group membership, regardless of designated laboratory status. The Group agreed to advertise the same information within their home organisations and external scientific networks.

10. After review, the MS subgroup recommended that the data under code 04-2-0617ar be moved to the Validation Group Working Database, since the data under code 04-2-0617a was previously accepted into the OCAD.

11. This document presents the sets of validated analytical data on scheduled chemicals recommended for inclusion in the OCAD (Annex 1). Validated analytical data on non-scheduled chemicals relevant to the Chemical Weapons Convention are found in Annex 2 to this Note. Annex 3 to this Note lists the members and evaluators from the Validation Group.

12. The available data from all analytical techniques will be sent to the Validation Group at least six weeks before its next scheduled meeting, which is proposed to take place on 10 and 11 April 2024 at the OPCW Centre for Chemistry and Technology (ChemTech Centre). The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 25 March 2024. The evaluators agreed to provide their individual data evaluations prior to the meeting and to come to the meeting prepared to finalise the evaluation of the analytical data provided to the Group. If travel to the ChemTech Centre is not possible, the evaluators may meet virtually.

Annexes:

Annex 1: Lists of Approved Data on Scheduled Chemicals Recommended for Inclusion in the OPCW Central Analytical Database

Annex 2: Lists of Approved Data on Non-scheduled Chemicals Relevant to the Chemical Weapons Convention and Recommended for Inclusion in the OPCW Central Analytical Database

Annex 3: List of Members of the Validation Group

Annex 1

LISTS OF APPROVED DATA ON SCHEDULED CHEMICALS RECOMMENDED FOR INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE

Note: In the "Decision" column of the tables that follow, "A" means "accepted" and "B" means "accepted subject to minor corrections".

TABLE 1: LIST OF APPROVED MS DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
28-2-0249	Diphenyl methylphosphonoselenoate	2.B.04	A
28-2-0332	Methyl-d3 N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0333	Methyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
28-2-0334	Methyl-d3 N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0335	Ethyl-d5 N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0337	Ethyl-d5 N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0338	Propyl N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0339	Propyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0340	Propyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0341	Isopropyl N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0342	Isopropyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0343	Isopropyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
28-2-0344	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
07-2-3551	Ethyl S-2-N-methyl-N-propylaminoethyl isopropylphosphonothiolate	1.A.03	A
07-2-3552	Ethyl S-2-N-isopropyl-N-methylaminoethyl isopropylphosphonothiolate	1.A.03	A

TABLE 2: LIST OF APPROVED GC(RI) DATA ON SCHEDULED CHEMICALS

Note: Under the "Column" heading for GC(RI) data, a "1" means an HP5 or an SE54 column, and a "2" means a DB-5MS column.

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision
28-4-0333r	Ethyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1797	A
28-4-0334	Methyl-d3 N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1507	A
28-4-0335	Methyl-d3 N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1599	A
28-4-0336	Methyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1746	A
28-4-0337	Methyl-d3 N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1740	A
28-4-0338	Ethyl-d5 N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1577	A
28-4-0339	Ethyl-d5 N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1652	A
28-4-0340	Ethyl-d5 N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1792	A
28-4-0341	Propyl N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1666	A
28-4-0342	Propyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1755	A
28-4-0343	Propyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1888	A
28-4-0344	Isopropyl N-(1-(dimethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1593	A
28-4-0345	Isopropyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1679	A
28-4-0346	Isopropyl N-(1-(dipropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1813	A
28-4-0347	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1523	A

TABLE 3: LIST OF APPROVED IR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
04-1-0354v	2-Methylcyclopentyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-1-0359v	1,1,2-Trimethylpropyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	B
04-1-0362v	1,1,2-Trimethylpropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B

TABLE 4: LIST OF APPROVED NMR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
05-3-0195	O-Isobutyl methylphosphonothionate, sodium salt	2.B.04	B
05-3-0196	O-Isobutyl methylphosphonothionate, sodium salt	2.B.04	B
05-3-0197	O-Isobutyl methylphosphonothionate, sodium salt	2.B.04	B
05-3-0198	Methylphosphonic fluoride	2.B.04	A
05-3-0199	Methylphosphonic fluoride	2.B.04	A
05-3-0200	Methylphosphonic fluoride	2.B.04	A
05-3-0201	Methylphosphonic fluoride	2.B.04	A
05-3-0202	Methylphosphonic fluoride	2.B.04	A
33-3-0011r	Ethyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	A

TABLE 5: LIST OF APPROVED MS/MS DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
35-5-0004	Diethyl phosphite	3.B.11	B
35-5-0005	Diethyl phosphite	3.B.11	B
35-5-0006	Diethyl phosphite	3.B.11	B
35-5-0007	Dimethyl ethylphosphonate	2.B.04	B
35-5-0008	Dimethyl ethylphosphonate	2.B.04	B
35-5-0009	Dimethyl ethylphosphonate	2.B.04	B
35-5-0010	O,O-Dimethyl ethylphosphonothionate	2.B.04	B
35-5-0011	O,O-Dimethyl ethylphosphonothionate	2.B.04	B
35-5-0012	O,O-Dimethyl ethylphosphonothionate	2.B.04	B

TABLE 6: LIST OF APPROVED GC–HRMS[1] DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
02-7-0001	Diethyl methylphosphonate	2.B.04	A
02-7-0002	Diisopropyl methylphosphonate	2.B.04	A
14-7-0006	Diisopropyl methylphosphonate	2.B.04	A

[1] GC-HRMS = gas chromatography-high resolution mass spectrometry.

Annex 2

LISTS OF APPROVED DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION AND RECOMMENDED FOR INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE

Note: In the "Decision" column of the tables that follow, an "A" means "accepted," and a "B" means "accepted subject to minor corrections".

TABLE: LIST OF APPROVED MS/MS DATA ON NON-SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision	Justification[2]
35-5-0001	Tributyl phosphate	NS	B	Standard
35-5-0002	Tributyl phosphate	NS	B	
35-5-0003	Tributyl phosphate	NS	B	

[2] MS/MS data is used only by the off-site laboratories.

Annex 3

LIST OF MEMBERS OF THE VALIDATION GROUP

Name	Country	Address	Phone/Fax/Email	Speciality
Christine Albaret[†]	France	DGA Maîtrise NRBC BP-3 91710 Vert-le-Petit, France	+33 1 69908224 +33 1 64935266 christine.albaret@intradef.gouv.fr	NMR
Armando Alcaraz[*]	United States of America	Lawrence Livermore National Laboratory Forensic Science Center P.O. Box 808, L-090 Livermore, CA 94550, United States of America	+1 925 423 6889 +1 925 423 9014 (fax) alcaraz1@llnl.gov	MS, IR Coordinator of the IR subgroup
Mehran Babri	Islamic Republic of Iran	Defence Chemical Research Lab (DCRL) P.O. Box 31585-1461 Karaj, Islamic Republic of Iran	+98 263 2313442 +98 263 2313447 (fax) dcrl.mod@gmail.com	MS
Adam Bosák[*]	Czech Republic	National Institute for NBC Protection (SÚJCHBO, v.v.i.) Chemical Protection Department Kamenná 71, 262 31 Milín, Czech Republic	+420 318 600 235 +420 318 626 055 (fax) bosak@sujchbo.cz	IR
Arkady Braun[*]	Russian Federation	LCAC 27th Research Centre of the Ministry of Defense, Russian Federation	+7 915 4558009 avbraun@yandex.ru	MS

[*] The evaluator was present at this meeting of the Group and provided a written evaluation.
[**] The evaluator attended the meeting virtually and provided a written evaluation.
[†] The evaluator provided a written evaluation but did not attend the meeting.
[#] The evaluator was present at the meeting but did not provide a written evaluation.

Name	Country	Address	Phone/Fax/Email	Speciality
Jan Dědič*	Czech Republic	National Institute for NBC Protection (SÚJCHBO, v.v.i.) Chemical Protection Department Kamenná 71, 262 31 Milín, Czech Republic	+420 318 600 235 +420 318 626 055 (fax) dedic@sujchbo.cz	IR
Zdeňka Fabiánová*	Czech Republic	State Office for Nuclear Safety Division of Chemical Weapons Prohibition Senovážné nám. 9, 110 00 Praha 1, Czech Republic	+420 226 514 372 zdenka.fabianova@sujb.cz	IR
Arne Ficks†	Germany	Wehrwissenschaftliches Institut für Schutztechnologien – ABC-Schutz (WIS) 29633 Munster, Germany	+49 5192 136 428 +49 5192 136 355 (fax) arneficks@bundeswehr.org	MS
Hanna Hakulinen*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki, Finland	+358 5037 67914 hanna.hakulinen@helsinki.fi	MS
Harri August Heikkinen†	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki, Finland	+358 2941 50448 harri.a.heikkinen@helsinki.fi	NMR
Karin Höjer Holmgren*	Sweden	FOI CBRN Defence and Security Cementvagen 20, SE-90182 Umeå, Sweden	+46 90 106665 +46 72 5709234 karin.hojer@foi.se	MS Coordinator of the MS subgroup
Karen Jacques	United Kingdom of Great Britain and Northern Ireland	DSTL Porton Down, Salisbury, SP4 0JQ, United Kingdom of Great Britain and Northern Ireland	+44 (0)1980 956645 kajacques@dstl.gov.uk	MS
Ethan Alex Jestel**	United States of America	DEVCOM CBC Forensic Analytical Center Maryland, United States of America	+1 410 436 0306 ethan.a.jestel.civ@army.mil	GC

Name	Country	Address	Phone/Fax/Email	Speciality
Matti Kuula*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki, Finland	+358 2941 50447 matti.kuula@helsinki.fi	GC
Shilei Liu**	China	RICD Yangfang Town, Changping District P.O. Box 1043, 102205 Beijing, China	+86 10 69760259 liushilei402@263.net	MS
Damian Magiera*	Germany	Wehrwissenschaftliches Institut für Schutztechnologien - ABC-Schutz (WIS) 29633 Munster, Germany	+49 5192 136 402 +49 5192 136 355 (fax) damianmagiera@bundeswehr.org	NMR, IR Coordinator of the NMR subgroup
Gary Mallard**	United States of America	Teal Consulting Chevy Chase, MD 20815, United States of America	+1 301 656-0402 gary.mallard@gmail.com	GC Coordinator of the GC subgroup
Brian Mayer*	United States of America	Lawrence Livermore National Laboratory 7000 East Avenue, L-091 Livermore, CA 94550, United States of America	+1 925 423 1128 +1 925 423 9014 (fax) mayer22@llnl.gov	NMR Chairperson of the Validation Group
Urs Meier†	Switzerland	Spiez Laboratory CH-3700 Spiez, Switzerland	+41 33228 1713 +41 33228 1402 urs.meier@babs.admin.ch	NMR
Mohammad Taghi Naseri	Islamic Republic of Iran	Defence Chemical Research Lab (DCRL) P.O. Box 31585-1461, Karaj, Islamic Republic of Iran	+98 263 2313442 +98 263 2313447 (fax) dcrl.mod@gmail.com	GC
Deepak Pardasani†	India	Defence Research & Development Establishment (DRDE) Jhansi Road, Gwalior-474002, India	+91 751 2341148 +91 751 2233488 dkpardasani@drde.drdo.in	GC

Name	Country	Address	Phone/Fax/Email	Speciality
Vijay Tak**	India	Defence Research & Development Establishment (DRDE) Jhansi Road, Gwalior-474002, India	+91 751 2233488 +91 751 2390314 takvijay.drde@gov.in	MS
Jijun Tang	China	AMMS 27 Taiping Road, Haidian District, Beijing, China	+8610 13810338946 tangjijun2012@163.com	GC
Dušan Trefilík#	Czech Republic	NBC Defence institute Vita Nejedleho 1, Vyskov, Czech Republic	+420 777 255 274 dusan.trefilik@seznam.cz	MS

- - - o - - -