OPCW

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NOTE BY THE TECHNICAL SECRETARIAT

REPORT OF THE FIFTY-FOURTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 21 – 22 SEPTEMBER 2022

1. The Validation Group met on 21 and 22 September 2022 to discuss the evaluation of new 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. The coordinators provided an evaluation summary of the data to the Validation Group for discussion at the meeting. The evaluators finalised the evaluation of the analytical data and confirmed that the approved data was technically valid.

4. Ms Karin Holmgren summarised the MS subgroup's ongoing discussion on the development of a dedicated GC high-resolution mass spectrometry (GC-HRMS) database for off-site analysis. To support this work, the subgroup drafted reporting requirements for GC-HRMS data for circulation among the Validation Group members.

5. The Validation Group affirmed previous discussions that MS and GC(RI) data for the same chemical should be accepted together to coordinate data submission and review. It was recommended that reviews of these data be performed by currently established subgroups and that a coordinated joint review be conducted, as needed.

6. The Validation Group recommended that abbreviations appearing in both the OCAD and the Validation Group Working Database (e.g., DSX, PS, etc.) be defined in a document to be supplied as part of future OCAD and Validation Group Working Database releases.

7. Mr Daan Noort (Netherlands), Mr Ferdinand Visser (South Africa), and Mr Devendra K. Dubey (India) announced their resignations from the Validation Group. They were recognised and thanked for their contributions to the Group and were wished well in their new roles.

8. This document presents the sets of validated analytical data on scheduled chemicals (Annex 1) recommended for inclusion in the OCAD. Validated analytical data on non-scheduled chemicals relevant to the Chemical Weapons Convention (hereinafter "the Convention") are found in Annex 2 to this Note. Validated analytical data on derivatised chemicals relevant to the Convention are summarised in Annex 3.

9. The Group discussed the derivatives data using 3,4-Dimercaptotoluene (DMT). It was agreed that these data are to be removed from the OCAD, as DMT is not approved for use during on-site inspections. It was suggested that the DMT derivatives should be categorised in "DSX", which would be exclusively contained within the Validation Group Working Database. Details of these derivatives data are listed in Annex 4 to this Note.

10. Annex 5 to this Note lists the members and evaluators from the Validation Group.

11. 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 29 and 30 March 2023. The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 23 March 2023. 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 OPCW Headquarters is not possible, the evaluators could 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: Lists of Approved Data on Derivatives Relevant to the Chemical Weapons Convention

Annex 4: Data Entries Recommended to Be Removed from the OPCW Central Analytical Database

Annex 5: 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
33-2-0001	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-2-0002	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-2-0003	Ethyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-2-0004	Methyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-2-0005	Ethyl N-(1-(isopropylmethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-2-0006	Ethyl N-(1-(ethylmethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-2-0008	Ethyl N-(1-(ethylmethylamino)propylidene)phosphoramidofluoridate	1.A.14	B

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
33-4-0001	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1662	A
33-4-0002	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1603	A
33-4-0003	Ethyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	1	1596	A
33-4-0004	Methyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	1	1537	A
33-4-0005	Ethyl N-(1-(isopropylmethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1673	A
33-4-0006	Ethyl N-(1-(ethylmethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1618	A
33-4-0007	Ethyl N-(1-(isopropylmethylamino)propylidene)phosphoramidofluoridate	1.A.14	1	1691	A
33-4-0008	Ethyl N-(1-(ethylmethylamino)propylidene)phosphoramidofluoridate	1.A.14	1	1639	A

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 1: LIST OF APPROVED MS DATA ON NON-SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision	Justification	Classification
31-2-0004	N,N-Dipropylethanimidamide	NS	A	Precursors of 1.A.14	NDP(1A14)*
31-2-0005	N,N-Dibutylethanimidamide	NS	A		
31-2-0008	N,N-Dipropylbutanimidamide	NS	A		
31-2-0009	N,N-Dimethylethanimidamide	NS	A		
31-2-0010	N,N-Dibutylpentanimidamide	NS	A		
32-2-0002	Bis[2-(N,N-diisopropylamino)ethyl]ether	NS	B	Reaction by-product of 1.A.03	NDP(1A03)**

* Non-scheduled precursors, degradation products, or known synthesis impurities or by-products related to schedule 1.A.14.
** Non-scheduled precursors, degradation products or known synthesis impurities or by-products related to schedule 1.A.03.

TABLE 2: LIST OF APPROVED GC(RI) DATA ON NON-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	Justification	Classification
31-4-0003	N,N-Diethylethanimidamide	NS	2	973	A	Precursor 1.A.14	NDP(1A14)*
31-4-0004	N,N-Dipropylethanimidamide	NS	2	1138	A		
31-4-0005	N,N-Dibutylethanimidamide	NS	2	1322	A		
31-4-0006	N,N-Diethylpropanimidamide	NS	2	1055	A		
31-4-0008	N,N-Dipropylbutanimidamide	NS	2	1288	A		
31-4-0009	N,N-Dimethylethanimidamide	NS	2	841	A		
31-4-0010	N,N-Dibutylpentanimidamide	NS	2	1553	A		
32-4-0002	Bis[2-(N,N-diisopropylamino)ethyl]ether	NS	1	1644	A	Reaction by-product of 1.A.03	NDP(1A03)**

* Non-scheduled precursors, degradation products, or known synthesis impurities or by-products related to schedule 1.A.14.
** Non-scheduled precursors, degradation products or known synthesis impurities or by-products related to schedule 1.A.03.

Annex 3

LISTS OF APPROVED DATA ON DERIVATIVES RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

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

TABLE 1: LIST OF APPROVED MS DATA ON DERIVATIVES

OPCW Code	Chemical Name	Schedule	Decision
31-2-0007	(Dimethyl(1,2,2-trimethylpropoxy)silyl)benzene	DSX	B

Note: This compound is a derivative of 3,3-Dimethylbutan-2-ol (2.B.14).

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

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
31-4-0007	(Dimethyl(1,2,2-trimethylpropoxy)silyl)benzene	DSX	2	1369	A

Note: This compound is a derivative of 3,3-Dimethylbutan-2-ol (2.B.14).

Annex 4

DATA ENTRIES RECOMMENDED TO BE REMOVED FROM THE OPCW CENTRAL ANALYTICAL DATABASE

OPCW Code(s)	Chemical Name	Justification
17-2-0092	2-Chloro-5-methyl-1,3,2-benzodithiarsole	DMT derivative of Arsenic trichloride (2.B.07)
06-2-0359		
17-4-0049		
17-2-0093	2-(2-Chlorovinyl)-5-methyl-1,3,2-benzodithiarsole	DMT derivative of 2-Chlorovinyldichloroarsine (1.A.05)
08-2-0090		
06-2-0358		
17-4-0050		

Note: 3,4-Dimercaptotoluene (DMT) is not approved for use during on-site inspections.

Annex 5

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