OPCW

Technical Secretariat

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NOTE BY THE TECHNICAL SECRETARIAT

REPORT OF THE FIFTY-NINTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 9 AND 10 APRIL 2025

1. The Validation Group met on 9 and 10 April 2025 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 videoconference. 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, along with the technique for which each was responsible, are listed below:

Mr Armando Alcaraz (United States of America)	Infrared (IR) spectroscopy
Mr Arkady Braun (Russian Federation) (Acting)	Mass spectrometry (MS)
Mr Damian Magiera (Germany)	Nuclear magnetic resonance (NMR) spectroscopy
Mr Marc-Michael Blum (Germany)	Gas chromatography (retention index) (GC(RI))

3. Ms Hoe Chee Chua (Singapore), Mr Petrus Hemström (Sweden), Mr Leong Yeow Benjamin Koh (Singapore), and Ms Arja Valtanen (Finland) joined the Validation Group and were acknowledged and welcomed by the existing members. Mr Jelle de Koning (Netherlands) and Mr Andrei Polezhaev (Russian Federation) were present as observers.

4. Ms Karin Höjer Holmgren (Sweden) resigned as MS subgroup coordinator and was thanked for her leadership and service in this role. Ms Hanna Hakulinen (Finland) resigned from the Validation Group and was also thanked for her service.

5. Mr Arkady Braun (Russian Federation) served as the acting MS subgroup coordinator for this meeting. An election was held to appoint a new MS subgroup coordinator, and Mr Braun was elected to the role by his fellow subgroup members after his nomination.

6. The Validation Group continues to actively recruit new members. Nominations for membership are welcomed by any member of the chemical sciences community with recognised expertise in the field of analytical chemistry. Prospective members are not required to work for an OPCW designated laboratory. Nominations are provided to the OPCW Technical Secretariat (the Secretariat) by the nominee's National Authority and must include a curriculum vitae confirming their expertise.

7. During the fifty-eighth meeting of the Validation Group, the Group decided to review approximately 350 previously evaluated data sets on non-scheduled chemicals not yet sent for approval by the OPCW Executive Council. This review started during the current meeting, focusing on IR and NMR data of compounds with previously accepted and distributed MS and GC(RI) data. Additional data will be reviewed as part of future Group meetings. Data deemed appropriate by the Group will be recommended for inclusion in the OCAD.

8. Building on previous discussions, the Validation Group explored new strategies to encourage additional submissions for potential inclusion in the OCAD. The Group decided to draft a document to communicate the Group's goal of expanding the OCAD to a wider audience. Additionally, the Group emphasised the importance of its members promoting data submissions at relevant scientific meetings and external conferences and reinforcing the message that any laboratory is welcome to submit data for consideration.

9. The Validation Group has agreed to identify and prioritise the data most crucial for expanding the OCAD, as a comprehensive analysis of this data has not been conducted since 2015. This effort will begin after the current meeting and will involve both Validation Group members and the OPCW Laboratory.

10. To simplify the data submission and evaluation processes and encourage new laboratories to participate, Validation Group members continued discussions on creating submission templates for each analytical technique. The Group agreed to collaborate within their subgroups to develop these templates before the next meeting. Once finalised, the templates will be incorporated into the official guidelines for data submission.

11. Following discussions at the fifty-eighth Validation Group meeting, the MS and GC(RI) subgroups initiated joint meetings after their individual sessions. This approach ensures data recommended for inclusion in the OCAD is thoroughly discussed and holistically evaluated.

12. The MS and GC(RI) subgroups decided that if an MS submission is evaluated as A or B, but the corresponding GC(RI) data is rejected, then the MS data will be postponed and the submitting laboratory will be asked to resubmit both GC(RI) and MS data. Additionally, if an MS data submission is rejected, then the corresponding GC(RI) data is also rejected. An exception can be made in the case of isomers with multiple RI values.

13. The Validation Group recommended that the OPCW Laboratory should check all postponed GC(RI) data, or those data evaluated as A or B yet not included in the OCAD. If corresponding MS data is absent, the Group recommends that this GC(RI) data be rejected.

14. If laboratories submit GC(RI) and MS data for compound classes lacking a significant amount of comparative data to substantiate a measured GC(RI) value and these data are rejected or postponed, then the Validation Group recommends a resubmission with supporting GC(RI) data from another GC instrument with an identical GC method. Laboratories may also provide additional data such as the compound's molecular ion measured by chemical ionisation or supporting gas chromatography high-resolution mass spectrometry (GC-HRMS) data to facilitate data evaluation.

15. The Validation Group has received submissions for compounds eluting after the OPCW GC-MS test mixture. While this requires submitting laboratories to extend the calibration range, it may also have implications for the use of GC-MS during the on-site sampling and analysis missions. The Group encourages the Secretariat to review these implications and identify practical solutions.

16. The MS subgroup discussed revising submission requirements related to spectral background subtraction. The Group suggested that ions with intensities ≤1% need not be considered during evaluation.

17. 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 were technically valid.

18. 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 Convention recommended for inclusion in the OCAD are found in Annex 2 to this Note. Annex 3 summarises other validated analytical data on non-scheduled chemicals relevant to the Convention currently not recommended for inclusion in the OCAD. Annex 4 summarises the MS and GC(RI) data entries recommended for removal from the OCAD. Annex 5 lists the members and evaluators of the Validation Group.

19. 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 17 and 18 September 2025 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 5 September 2025, and 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: Lists of Approved Data on Non-scheduled Chemicals Relevant to the Chemical Weapons Convention

Annex 4: Lists of Data Entries Recommended for Removal 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
04-2-0659	Cyclopentyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0660b	2-Methylcyclopentyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A
05-2-0206	N-(Bis(diethylamino)methylidene)-P-methylphosphonamidic fluoride	1.A.15	A
05-2-0208	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
07-2-3608	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
07-2-3609	N-(1-(Dibutylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
07-2-3610	N-(1-(Dioctylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
07-2-3611	N-(1-(Diethylamino)ethylidene)-P-pentylphosphonamidic fluoride	1.A.13	A
07-2-3612	N-(1-(Dipropylamino)ethylidene)-P-pentylphosphonamidic fluoride	1.A.13	A
07-2-3613	N-(1-(Dibutylamino)ethylidene)-P-pentylphosphonamidic fluoride	1.A.13	A
07-2-3615	N-(1-(Diethylamino)ethylidene)-P-hexylphosphonamidic fluoride	1.A.13	A
07-2-3616	N-(1-(Dipropylamino)ethylidene)-P-hexylphosphonamidic fluoride	1.A.13	A
07-2-3617	N-(1-(Dibutylamino)ethylidene)-P-hexylphosphonamidic fluoride	1.A.13	A
07-2-3619	N-(1-(Diethylamino)ethylidene)-P-octylphosphonamidic fluoride	1.A.13	A
07-2-3620	N-(1-(Dipropylamino)ethylidene)-P-octylphosphonamidic fluoride	1.A.13	A

OPCW Code	Chemical Name	Schedule	Decision
07-2-3621	N-(1-(Dibutylamino)ethylidene)-P-octylphosphonamidic fluoride	1.A.13	A
07-2-3623	N-(1-(Diethylamino)ethylidene)-P-decylphosphonamidic fluoride	1.A.13	A
07-2-3624	N-(1-(Dipropylamino)ethylidene)-P-decylphosphonamidic fluoride	1.A.13	A
07-2-3625	N-(1-(Dibutylamino)ethylidene)-P-decylphosphonamidic fluoride	1.A.13	A
29-2-0019r	Methyl N-(1-(dibutylamino)ethylidene)phosphoramidofluoridate	1.A.14	A

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

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

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	Decision
04-4-0468	Cyclopentyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	1	1670		A
04-4-0469	2-Methylcyclopentyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	1	1698	1702	A
05-4-0212	N-(Bis(diethylamino)methylidene)-P-methylphosphonamidic fluoride	1.A.15	2	1653		A
05-4-0214	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	2	1662		A
07-4-3471	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	2	1650		A
07-4-3472	N-(1-(Dibutylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	2	1830		A
07-4-3473	N-(1-(Dioctylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	2	2607		A
07-4-3474	N-(1-(Diethylamino)ethylidene)-P-pentylphosphonamidic fluoride	1.A.13	2	1881		A
07-4-3475	N-(1-(Dipropylamino)ethylidene)-P-pentylphosphonamidic fluoride	1.A.13	2	2019		A
07-4-3476	N-(1-(Dibutylamino)ethylidene)-P-pentylphosphonamidic fluoride	1.A.13	2	2187		A
07-4-3478	N-(1-(Diethylamino)ethylidene)-P-hexylphosphonamidic fluoride	1.A.13	2	1984		A

07-4-3479	N-(1-(Dipropylamino)ethylidene)-P-hexylphosphonamidic fluoride	1.A.13	2	2119		A
07-4-3480	N-(1-(Dibutylamino)ethylidene)-P-hexylphosphonamidic fluoride	1.A.13	2	2285		A
07-4-3482	N-(1-(Diethylamino)ethylidene)-P-octylphosphonamidic fluoride	1.A.13	2	2193		A
07-4-3483	N-(1-(Dipropylamino)ethylidene)-P-octylphosphonamidic fluoride	1.A.13	2	2326		A
07-4-3484	N-(1-(Dibutylamino)ethylidene)-P-octylphosphonamidic fluoride	1.A.13	2	2489		A
07-4-3486	N-(1-(Diethylamino)ethylidene)-P-decylphosphonamidic fluoride	1.A.13	2	2404		A
07-4-3487	N-(1-(Dipropylamino)ethylidene)-P-decylphosphonamidic fluoride	1.A.13	2	2535		A
07-4-3488	N-(1-(Dibutylamino)ethylidene)-P-decylphosphonamidic fluoride	1.A.13	2	2695		A
29-4-0019	Methyl N-(1-(dibutylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1922		A
29-4-0020	Methyl N-(1-(dipropylamino)butylidene)phosphoramidofluoridate	1.A.14	1	1799		A
29-4-0021	Methyl N-(1-(dibutylamino)butylidene)phosphoramidofluoridate	1.A.14	1	1963		A

TABLE 3: LIST OF APPROVED GC-HRMS DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
29-7-0006r	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0018r	O-Methyl S-cyclohexyl methylphosphonothiolate	2.B.04	A
29-7-0019r	O-Methyl S-hexyl methylphosphonothiolate	2.B.04	A
29-7-0020r	O-Methyl S-heptyl methylphosphonothiolate	2.B.04	A
29-7-0026r	O-Ethyl S-heptyl methylphosphonothiolate	2.B.04	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, "A" means "accepted," and "B" means "accepted subject to minor corrections".

TABLE 1: LIST OF APPROVED IR DATA ON NON-SCHEDULED CHEMICALS[1]

OPCW Code	Chemical Name	Schedule	Decision	Justification
09-1-0014	N,N-Dimethyl-N-(2-trimethylsilyloxyethyl)amine[2]	NS	B	TMS derivative of N,N-dimethylaminoethanol. Exempted in 2.B.11, but a degradation product of 1.A.03 chemicals
19-1-0014	Tris(2-chloroethyl)amine hydrochloride[3]	PS	A	Protonated salt of 1.A.06
19-1-0023x	2-Chloroacetophenone[4]	NS	A	Riot control agent as established in SAB-25/WP.1 (dated 27 March 2017)
19-1-0030x	Pelargonic acid vanillylamide[5]	NS	A	Riot control agent as established in SAB-25/WP.1

1 Data previously evaluated during the nineteenth, thirty-fourth, and thirty-sixth Validation Group meetings and re-evaluated during the fifty-ninth Validation Group meeting.

2 Chemical accepted into OCAD_v20_2018 as MS data (07-2-3033) and GC(RI) data (07-4-2796) (decision EC-86/DEC.10, dated 13 October 2017).

3 Chemical accepted into OCAD_v6v8 as IR data (08-1-0199) and NMR data (06-3-0215, 06-3-0217, 07-3-0179, 07-3-0180) (decision C-I/DEC.64, dated 22 May 1997 and Corr.1, dated 13 October 1997).

4 Chemical accepted into OCAD_v20_2018 as MS data (16-2-0018) and GC(RI) data (16-4-0047 and 19-4-0007) (EC-86/DEC.10).

5 Chemical accepted into OCAD_v20_2018 as MS data (25-2-0018) and GC(RI) data (24-4-0057r) (EC-86/DEC.10).

TABLE 2: LIST OF APPROVED MS DATA ON NON-SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision	Justification	Classification
04-2-0653	Methyl N-(1-(diethylamino)ethylidene)phosphoramidochloridate	NS	B	Reaction by-product, precursor, or degradation product of 1.A.14	NDP-N[6]
04-2-0655	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidochloridate	NS	A		
04-2-0657	N-(1-(Diethylamino)ethylidene)phosphoramidic difluoride	NS	A		
04-2-0658	N-(1-(Diethylamino)ethylidene)phosphoramidic dichloride	NS	B		
05-2-0202	N,N-Diethyl-N'-(trimethylsilyl)acetimidamide	NS	A	Precursor of 1.A.13 and 1.A.14	NDP-N
05-2-0203	N,N-Dipropyl-N'-(trimethylsilyl)acetimidamide	NS	A		
05-2-0204	N-Methyl-N-propyl-N'-(trimethylsilyl)acetimidamide	NS	A		
05-2-0205	N,N,N',N'-Tetraethyl-N''-(trimethylsilyl)guanidine	NS	A	Precursor of 1.A.15	NDP-N

[6] Non-scheduled precursors, degradation products, known synthesis impurities, or by-products related to Schedules 1.A.13, 1.A.14, 1.A.15, and 1.A.16.

TABLE 3: LIST OF APPROVED GC(RI) DATA ON NON-SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision	Justification	Classification
04-4-0462	Methyl N-(1-(diethylamino)ethylidene)phosphor-amidochloridate	NS	1	1793	B	Reaction by-product, precursor, or degradation product of 1.A.14	NDP-N
04-4-0464	Ethyl N-(1-(diethylamino)ethylidene)phosphor-amidochloridate	NS	1	1842	A		
04-4-0466	N-(1-(Diethylamino)ethylidene)phosphoramidic difluoride	NS	1	1421	A		
04-4-0467	N-(1-(Diethylamino)ethylidene)phosphoramidic dichloride	NS	1	1825	A		
05-4-0208	N,N-Diethyl-N'-(trimethylsilyl)acetimidamide	NS	2	1127	A	Precursor of 1.A.13 and 1.A.14	NDP-N
05-4-0209	N,N-Dipropyl-N'-(trimethylsilyl)acetimidamide	NS	2	1265	A		
05-4-0210	N-Methyl-N-propyl-N'-(trimethylsilyl)acetimidamide	NS	2	1156	A		
05-4-0211	N,N,N',N' -Tetraethyl-N''-(trimethylsilyl)guanidine	NS	2	1312	A	Precursor of 1.A.15	NDP-N

Annex 3

LISTS OF APPROVED DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

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 IR DATA ON NON-SCHEDULED CHEMICALS[7]

OPCW Code	Chemical Name	Schedule	Decision
02-1-0092	Dioctyl N,N-dimethylphosphoramidate	NS	B
02-1-0094	Dihexyl N,N-dimethylphosphoramidate	NS	B
02-1-0230	Tetrakis(2-chlorovinyl)diarsoxane	NS	B
02-1-0232	Diethyl (2-chlorovinyl)arsonite	NS	B
02-1-0235	Propyl bis(2-chlorovinyl)arsinothiolite	NS	B
02-1-0236	Pinacolyl (2-chlorovinyl)arsonochloridite	NS	B
02-1-0239	Decyl bis(2-chlorovinyl)arsinite	NS	B
02-1-0240	Pinacolyl bis(2-chlorovinyl)arsinite	NS	B
02-1-0241	Octyl bis(2-chlorovinyl)arsinite	NS	B
02-1-0242	Octyl 2-chlorovinylarsonochloridite	NS	B
02-1-0244	Decyl 2-chlorovinylarsonochloridite	NS	B
02-1-0245	2-Methoxy-2-oxoethyl bis(2-chlorovinyl)arsinothiolite	NS	B
02-1-0246	Bis(2-methoxy-2-oxoethyl) (2-chlorovinyl)arsonodithiolite	NS	B
19-1-0026x	10-Chloro-5,10-dihydrophenarsazine	NS	A
19-1-0027x	Benzyl bromide	NS	A

TABLE 2: LIST OF APPROVED MS DATA OF DERIVATISED CHEMICALS RELEVANT TO THE CONVENTION

OPCW Code	Chemical Name	Schedule	Decision
05-2-0209	Pinacolyl heptafluorobutanoate	DSX[8]	A

[7] Data previously evaluated during the twenty-fifth, twenty-ninth, and thirty-fourth Validation Group meetings and re-evaluated during the fifty-ninth Validation Group Meeting.

[8] Derivative of scheduled chemical (another derivatisation agent than BSTFA or BuSH).

TABLE 3: LIST OF APPROVED GC(RI) DATA OF DERIVATISED CHEMICALS RELEVANT TO THE CONVENTION

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision
05-4-0215	Pinacolyl heptafluorobutanoate	DSX	2	839	A
17-4-0230	Pinacolyl heptafluorobutanoate	DSX	1	849	A

Annex 4

LISTS OF DATA ENTRIES RECOMMENDED FOR REMOVAL FROM THE OPCW CENTRAL ANALYTICAL DATABASE

TABLE 1: LIST OF DUPLICATE MS DATA RECOMMENDED FOR REMOVAL FROM THE OCAD

OPCW Code	Chemical Name	Schedule
04-2-0552	2-Ethylhexyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03
04-2-0553	Nonyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03
04-2-0554	1-Methyloctyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03
04-2-0555	Decyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03
04-2-0556	1-Methylnonyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03
04-2-0580	1-Ethylpropyl N,N-dimethylphosphoramidocyanidate	1.A.02

TABLE 2: LIST OF DUPLICATE GC(RI) DATA RECOMMENDED FOR REMOVAL FROM THE OCAD

OPCW Code	Chemical Name	Schedule
04-4-0389	1-Ethylpropyl N,N-dimethylphosphoramidocyanidate	1.A.02
17-4-0207	(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate	2.B.04
28-4-0326	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13

Annex 5

LIST OF MEMBERS OF THE VALIDATION GROUP

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[*] The evaluator was present at this meeting of the Validation Group (either in person or virtually) and provided a written evaluation.
[†] The evaluator provided a written evaluation but did not attend the meeting.
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