



NOTE BY THE TECHNICAL SECRETARIAT

**REPORT OF THE FIFTY-FIFTH MEETING OF THE VALIDATION GROUP FOR
THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE
4 – 5 APRIL 2023**

1. The Validation Group met on 4 and 5 April 2023 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 Höjer 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. The subgroup presented finalised submission and evaluation criteria for GC-HRMS data for approval by the Validation Group members. The Group recommends to the Technical Secretariat that it include the criteria for GC-HRMS data in the guidelines for the submission and evaluation of data to be included in the OCAD.



5. The IR subgroup discussed issues regarding the IR DX data for submissions 05-1-0176 to 05-1-0187. The subgroup decided that the poor quality of the .dx files requires reformatting of the data.
6. The NMR subgroup discussed data sets 05-3-0088 and 05-3-0089. The subgroup concluded that chemical shifts in the carbon-13 spectrum (05-3-0089) are misassigned, requiring the data set currently in the OCAD to be revised.
7. Mr Leo de Reuver (Netherlands) announced his resignation from the Validation Group. He was recognised and thanked for his contributions to the Group and was wished well in retirement.
8. Mr Tomas van Groningen (Netherlands), Ms Anne Puustinen (Finland), Mr Matti Kuula (Finland), and Mr Vijay Tak (India) joined the Validation Group and were acknowledged and welcomed by the existing members. Ms Vladislava Talandova (Czech Republic), Mr Matthias Berger (Germany), Mr Dehghan Pir (Islamic Republic of Iran), Ms Elodie Jobard (France), and Ms Jina Wu (China) acted as observers for this Validation Group meeting.
9. This document presents the sets of validated analytical data on scheduled chemicals recommended for inclusion in the OCAD (Annex 1).
10. Annex 2 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 13 and 14 September 2023 at the new OPCW Centre for Chemistry and Technology (ChemTech Centre). The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 1 September 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 ChemTech Centre 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: 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
04-2-0636	2-Ethylhexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0637a	1,4-Dimethylpentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0637b	1,4-Dimethylpentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0639a	2-Methylcyclopentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0639b	2-Methylcyclopentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	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)	RI(b)	Decision
04-4-0441	2,2-Dimethylpropyl N-isopropyl N-methylphosphoramidocyanidate	1.A.02	1	1432		A
04-4-0442	1-Ethylpropyl N-isopropyl N-methylphosphoramidocyanidate	1.A.02	1	1475		A
04-4-0445	2-Ethylhexyl N-isopropyl N-methylphosphoramidocyanidate	1.A.02	1	1753		A
04-4-0448	2-Methylcyclopentyl N-isopropyl N-methylphosphoramidocyanidate	1.A.02	1	1620	1635	A

TABLE 3: LIST OF APPROVED IR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
04-1-0444v	2,2-Dimethylpropyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-1-0445v	1-Ethylpropyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-1-0447v	Pinacolyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-1-0448v	2-Ethylhexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
04-1-0449v	1,4-Dimethylpentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-1-0450v	1-Isopropyl-2-methylpropyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
04-1-0451v	2-Methylcyclopentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
04-1-0453v	4-tert-Butylcyclohexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A

TABLE 4: LIST OF APPROVED NMR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
33-3-0003	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-3-0004	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-3-0005	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-3-0008	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-3-0009	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
33-3-0010	Ethyl N-(1-(diethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-3-0013	Ethyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-3-0014	Ethyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-3-0015	Ethyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-3-0018	Methyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-3-0019	Methyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B
33-3-0020	Methyl N-(1-(dimethylamino)propylidene)phosphoramidofluoridate	1.A.14	B

Annex 2

LIST OF MEMBERS OF THE VALIDATION GROUP

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¹ The evaluator attended the meeting virtually.

² The evaluator was present at this meeting of the Group.

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³ The evaluator provided an evaluation but did not attend the meeting.

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