OPCW **Technical Secretariat**

Verification Division
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REPORT OF THE TWENTY-SIXTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 18 AND 19 SEPTEMBER 2007

1. The Validation Group (hereinafter the "Group") met for the 26th time on 18 and 19 September 2007 to discuss the evaluation of new analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD), and to consider matters related to it. Mr Hugh Gregg of the United States of America chaired the Meeting.

2. The evaluators for the analytical techniques evaluated new data and sent their written reports 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 is responsible, are listed below:

Gas chromatography (retention index) GC(RI)	Mr Martin Söderström (Finland)
Mass spectrometry (MS)	Mr Vesa Häkkinen (Finland) Ms Sally Swindlehurst (United Kingdom of Great Britain and Northern Ireland)
Nuclear magnetic resonance spectrometry (NMR)	Mr Lars-Gunnar Hammarström (Sweden)

3. These coordinators provided an evaluation summary to the Group for discussion at the Meeting. The evaluators finalised the evaluation of the analytical data and confirmed that the data approved are technically valid.

4. The Group forwarded lists of the validated analytical data to the Director-General for appropriate action (see Annexes 1 and 2).

5. The Technical Secretariat (hereinafter "the Secretariat") reported that the data on scheduled chemicals submitted by the Validation Group after its 24th meeting to the Executive Council (hereinafter "the Council") for a decision at its Forty-Ninth Session had been approved, and that data from the 25th Validation Group meeting will be considered at a future Council meeting.

6. The Secretariat reported that a Validation Group Working Database (VGWD) is being prepared for the Group by the end of 2007. It was noted that this VGWD will be made available by the Secretariat on request.

7. The Group considered the fact that 12 infrared (IR) data in the OCAD are not in electronic format. The Group recommended not converting the existing spectra into electronic form, and reiterated the Secretariat's request to the contributing laboratories to submit new IR spectra for the subset of spectra for which electronic spectra do not currently exist in the OCAD.

8. The Group requested that the Secretariat submit the electronic files for the IR data to the IR coordinator for authentication.

9. The Group discussed the possibility of establishing a liquid chromatography-mass spectrometry (LC-MS) database for potential inclusion in the OCAD. Mr Martin Söderström summarised the efforts that had been made so far, and agreed to lead a subcommittee to explore the issue further. This subcommittee decided to start collecting sample data on eight selected chemicals that were appropriate for LC-MS analysis.

10. The Group noted the statement made by the International Union of Pure and Applied Chemistry (IUPAC) in paragraph 45 its report entitled *Impact of Scientific Developments on the Chemical Weapons Convention.* In that report, the IUPAC stated the following: "With regard to on-site analysis, the main gap is the absence of non-scheduled chemicals from the OCAD database." The Group discussed the issue of validation of non-scheduled chemicals, and agreed to continue to evaluate this class of chemicals provided that they are relevant to the Convention; this would include, for example, chemicals recommended by the Scientific Advisory Board.

11. The Group reviewed existing data in the OCAD, and recommended the removal of the data listed in Table 1 of Annex 3 (annexed hereto), since data of higher quality are available in the OCAD. Additionally, the Group requested that several typographical errors in the OCAD listed in Table 2 of Annex 3 be corrected.

12. The discussion, which was begun at the 21st meeting of the Group, on predicting GC(RI) data for those compounds for which the database has MS data only was continued. It was agreed that predictions presented at this Meeting, and which were based on existing data in the OCAD, will be evaluated at the 27th Meeting. For each chemical for which predicted data are accepted and subsequent experimental data are approved, the actual experimental data will automatically replace the predicted data in the OCAD.

13. The Group discussed acceptance criteria for GC(RI) data which have been obtained from a single GC-run. The information on the accuracy of measurements required by evaluation criteria could be obtained from repeated observations of quality control sample compounds.

14. The Group recommended that, if it requests a laboratory to resubmit data, the laboratory is to be encouraged to understand the changes requested by the Group. If the laboratory has questions in this regard, they are encouraged to seek clarification from the coordinator of the subgroup that evaluated the data.

15. The following new analytical data are available for evaluation at the next meeting:

MS	New Spectra	09-2-0121, 09-2-0122, 14-2-0110, 14-2-0111

16. Additional data are expected for NMR, MS, GC(RI), and IR before the end of the year.

17. Annex 4 to this report lists the evaluators by analytical technique. The evaluators agreed to send their written evaluation reports to the appointed coordinators **no later than 19 February 2008**. The coordinators agreed to send evaluation summary reports to the Group's Chairperson and to the evaluators **no later than 4 March 2008**, so that the reports can be discussed at the Group's next meeting, which is scheduled to take place on 11 and 12 March 2008. The evaluators agreed to come to that meeting prepared to finalise the evaluation of the analytical data referred to in paragraphs 15 and 16.

18. The Group welcomed Mr Mehran Babri (Islamic Republic of Iran) as a new evaluator for MS data, and Mr Damian Magiera (Germany) as a new evaluator for NMR data.

19. The Group noted its appreciation for the dedication, diligence, and hard work of Mr Edward White, former coordinator for MS data, and regrets that he is no longer able to participate and serve as coordinator for this group. The Group further notes the retirement of Mr Danian Xu, and expresses its appreciation for his work as a member of the MS group.

Annexes:

Annex 1: Lists of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
Annex 2: List of Technically Valid Data Not Recommended for Inclusion in the OPCW Central Analytical Database
Annex 3: Lists of Recommended Changes to the OPCW Central Analytical Database
Annex 4: List of Evaluators by Analytical Technique

Annex 1

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

Note: In the last column of the tables that follow in this and the next Annex, "A" means "accepted"; "B", "accepted subject to minor corrections". A "1" under the "Column" heading means an HP5 or an SE54 column.

TABLE 1: LIST OF APPROVED MS DATA

OPCW Code	Chemical Name	Schedule	Decision
07-2-1930	2-Dipropylaminoethyl methylphosphonofluoridate	2.B.04	B
07-2-1931	2-Diisopropylaminoethyl methylphosphonofluoridate	2.B.04	A
07-2-2350	O-Cyclobutyl methylphosphonothionochloridate	2.B.04	A
07-2-2385	N,N-Dipropylphosphoramidic difluoride	2.B.05	A
09-2-0113	2-Methyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
09-2-0114	2-Ethyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
09-2-0115	2-Isopropyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
09-2-0116	2-Propyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
09-2-0118	2-Ethyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
09-2-0119	2-Isopropyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
09-2-0120	2-Propyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
14-2-0032r	1-Ethyl-2-methylpropyl isopropylphosphonofluoridate	1.A.01	A
14-2-0038r	Decyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	A
14-2-0040r	Heptyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
14-2-0043r	1-Ethylpropyl S-2-diisopropylaminoethyl ethylphosphonothiolate	1.A.03	A
14-2-0045r	Decyl S-2-diisopropylaminoethyl ethylphosphonothiolate	1.A.03	A
14-2-0076r	2,6-Dimethylcyclohexyl methyl propylphosphonate	2.B.04	A
14-2-0098r	Sulfur dichloride	3.B.13	B
14-2-0099r	Sulfur monochloride	3.B.12	B
14-2-0100	2-Diisopropylaminoethyl ethylphosphonofluoridate	2.B.04	A
14-2-0101	2-Diisopropylaminoethyl isopropylphosphonofluoridate	2.B.04	A
14-2-0102	Bis(1-ethyl-2,2-dimethylpropyl) isopropylphosphonate	2.B.04	A
14-2-0103	Bis(1-ethylhexyl) dipropylpyrophosphonate	2.B.04	A
14-2-0105	3-Methylbutyl S-2-dipropylaminoethyl methylphosphonothiolate	1.A.03	A
14-2-0106	3-Methylbutyl S-2-dipropylaminoethyl ethylphosphonothiolate	1.A.03	A
14-2-0107	5-Isopropyl-2-methylcyclohexyl S-2-dimethylaminoethyl ethylphosphonothiolate	1.A.03	A
14-2-0108	O-Ethyl O-2-ethylthioethyl methylphosphonothionate	2.B.04	A
14-2-0109	O-Isopropyl O-trimethylsilyl propylphosphonothionate	2.B.04	A
16-2-0028	sec-Butyl isopropyl methylphosphonate	2.B.04	B
16-2-0029	sec-Butyl propyl methylphosphonate	2.B.04	B
16-2-0030	Butyl sec-butyl methylphosphonate	2.B.04	B
16-2-0031	Isobutyl isopropyl methylphosphonate	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
16-2-0032	Isobutyl propyl methylphosphonate	2.B.04	B
16-2-0033	Butyl isobutyl methylphosphonate	2.B.04	B
16-2-0034	sec-Butyl isobutyl methylphosphonate	2.B.04	B
16-2-0035	Isopropyl propyl ethylphosphonate	2.B.04	B
16-2-0036	Butyl isopropyl ethylphosphonate	2.B.04	B
16-2-0037	Butyl propyl ethylphosphonate	2.B.04	B
16-2-0038	sec-Butyl isopropyl ethylphosphonate	2.B.04	B
16-2-0039	sec-Butyl propyl ethylphosphonate	2.B.04	B
16-2-0040	Butyl sec-butyl ethylphosphonate	2.B.04	B
16-2-0041	Isobutyl isopropyl ethylphosphonate	2.B.04	B
16-2-0042	Isobutyl propyl ethylphosphonate	2.B.04	B
16-2-0043	Butyl isobutyl ethylphosphonate	2.B.04	B
16-2-0044	sec-Butyl isobutyl ethylphosphonate	2.B.04	B
16-2-0045	2-Methoxyethyl methyl propylphosphonate	2.B.04	B
16-2-0046	2-Methoxyethyl propyl propylphosphonate	2.B.04	B
16-2-0047	sec-Butyl isopropyl propylphosphonate	2.B.04	B
16-2-0048	sec-Butyl propyl propylphosphonate	2.B.04	B
16-2-0050	Butyl sec-butyl propylphosphonate	2.B.04	B
16-2-0051	Isobutyl isopropyl propylphosphonate	2.B.04	B
16-2-0052	Isobutyl propyl propylphosphonate	2.B.04	B
16-2-0053	Isobutyl 2-methoxyethyl propylphosphonate	2.B.04	B
16-2-0055	sec-Butyl isobutyl propylphosphonate	2.B.04	B
16-2-0056	Isopropyl 2-methoxyethyl propylphosphonate	2.B.04	B
16-2-0057	Bis(2-methoxyethyl) propylphosphonate	2.B.04	B
16-2-0058	Butyl 2-methoxyethyl propylphosphonate	2.B.04	B
16-2-0059	Ethyl 2-methoxyethyl propylphosphonate	2.B.04	B
27-2-0002	Ethyl isobutyl methylphosphonodithiolothionate	2.B.04	A
27-2-0003	Diisopropyl methylphosphonodithiolothionate	2.B.04	A
27-2-0004	Dipropyl methylphosphonodithiolothionate	2.B.04	A
27-2-0005	Ethyl propyl methylphosphonodithiolothionate	2.B.04	A
27-2-0006	Diisobutyl methylphosphonodithiolothionate	2.B.04	B
27-2-0007	Diethyl methylphosphonodithiolothionate	2.B.04	A
27-2-0008	Butyl ethyl methylphosphonodithiolothionate	2.B.04	A
27-2-0009	Ethyl isopropyl methylphosphonodithiolothionate	2.B.04	A
27-2-0010	Dibutyl methylphosphonodithiolothionate	2.B.04	A

TABLE 2: LIST OF APPROVED GC(RI) DATA

OPCW Code	Chemical Name	Schedule	Column	a	b	Decision
16-4-0067	sec-Butyl isopropyl methylphosphonate	2.B.04	1	1166	1168	A
16-4-0068	sec-Butyl propyl methylphosphonate	2.B.04	1	1227	1231	A
16-4-0069	Butyl sec-butyl methylphosphonate	2.B.04	1	1316	1321	B

OPCW Code	Chemical Name	Schedule	Column	a	b	Decision
16-4-0070	Isobutyl isopropyl methylphosphonate	2.B.04	1	1184		A
16-4-0071	Isobutyl propyl methylphosphonate	2.B.04	1	1247		A
16-4-0072	Butyl isobutyl methylphosphonate	2.B.04	1	1338		A
16-4-0073	sec-Butyl isobutyl methylphosphonate	2.B.04	1	1276	1280	A
16-4-0074	Isopropyl propyl ethylphosphonate	2.B.04	1	1209		A
16-4-0075	Butyl isopropyl ethylphosphonate	2.B.04	1	1299		A
16-4-0076	Butyl propyl ethylphosphonate	2.B.04	1	1364		A
16-4-0077	sec-Butyl isopropyl ethylphosphonate	2.B.04	1	1239	1242	A
16-4-0078	sec-Butyl propyl ethylphosphonate	2.B.04	1	1301	1306	A
16-4-0079	Butyl sec-butyl ethylphosphonate	2.B.04	1	1390	1396	A
16-4-0080	Isobutyl isopropyl ethylphosphonate	2.B.04	1	1259		A
16-4-0081	Isobutyl propyl ethylphosphonate	2.B.04	1	1322		A
16-4-0082	Butyl isobutyl ethylphosphonate	2.B.04	1	1412		A
16-4-0083	sec-Butyl isobutyl ethylphosphonate	2.B.04	1	1351	1356	A
16-4-0084	2-Methoxyethyl methyl propylphosphonate	2.B.04	1	1317		A
16-4-0085	2-Methoxyethyl propyl propylphosphonate	2.B.04	1	1458		A
16-4-0086	sec-Butyl isopropyl propylphosphonate	2.B.04	1	1313	1315	A
16-4-0087	sec-Butyl propyl propylphosphonate	2.B.04	1	1377	1381	A
16-4-0088	sec-Butyl 2-methoxyethyl propylphosphonate	2.B.04	1	1479	1484	A
16-4-0089	Butyl sec-butyl propylphosphonate	2.B.04	1	1465	1469	A
16-4-0090	Isobutyl isopropyl propylphosphonate	2.B.04	1	1334		A
16-4-0091	Isobutyl propyl propylphosphonate	2.B.04	1	1398		A
16-4-0092	Isobutyl 2-methoxyethyl propylphosphonate	2.B.04	1	1505		A
16-4-0093	Butyl isobutyl propylphosphonate	2.B.04	1	1487		B
16-4-0094	sec-Butyl isobutyl propylphosphonate	2.B.04	1	1425	1429	A
16-4-0095	2-Methoxyethyl propyl methylphosphonate	2.B.04	1	1308		A

Annex 2

LIST OF TECHNICALLY VALID DATA NOT RECOMMENDED FOR INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE

TABLE 1: LIST OF TECHNICALLY VALID MS DATA

OPCW Code	Chemical Name	Schedule	Decision
09-2-0103	Methyl N,N-dimethylaminoethyl-2-sulfonate	NS	B
09-2-0104	Methyl N-ethyl-N-methylaminoethyl-2-sulfonate	NS	B
09-2-0105	Methyl N,N-diethylaminoethyl-2-sulfonate	NS	B
09-2-0106	Methyl N-methyl-N-propylaminoethyl-2-sulfonate	NS	B
09-2-0107	Methyl N-isopropyl-N-methylaminoethyl-2-sulfonate	NS	B
09-2-0108	Methyl N-ethyl-N-isopropylaminoethyl-2-sulfonate	NS	B
09-2-0110	Methyl N,N-dipropylaminoethyl-2-sulfonate	NS	B
09-2-0111	Methyl N,N-diisopropylaminoethyl-2-sulfonate	NS	B
09-2-0112	Methyl N-isopropyl-N-propylaminoethyl-2-sulfonate	NS	B

B = Accepted; subject to minor corrections

Annex 3

LISTS OF RECOMMENDED CHANGES TO THE OPCW CENTRAL ANALYTICAL DATABASE

TABLE 1: LIST OF DATA TO REMOVE FROM THE OCAD

OPCW Code	Chemical Name	Schedule
08-1-0205	Cyanogen chloride	3.A.02
04-2-0374	Diisopropyl methylphosphonate	2.B.04

TABLE 2: LIST OF DATA TO CHANGE IN THE OCAD

OPCW Code	Chemical Name	Schedule	Action
04-2-0259	Diethyl N-methyl-N-isopropylphosphoramidate	2.B.06	Remove incorrect accelerating voltage from pdf file
04-4-0218	1-Methylpentyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	Change RI indices to 1868, 1874
04-4-0219	2-Methylpentyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	Change RI index to 1919

Annex 4

LIST OF EVALUATORS BY ANALYTICAL TECHNIQUE[1]

TABLE 1: IR EVALUATORS

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Colin Pottage	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury, Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 613397 +44 1980 613830 cpottage@dstl.gov.uk	**IR Coordinator** NMR
Martin Söderström	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 19150438 +358 9 19150437 martin.soderstrom@helsinki.fi	GC, IR
Steven Choquette	United States of America	NIST 100 Bureau Drive Stop 8312 Gaithersburg, MD 20899-8312 United States of America	+1 301 975 3096 +1 301 977 0587 steven.choquette@nist.gov	IR
Vladimir Podborsky	Czech Republic	MTIP Brno, Veslarskâ 230 P.O. Box 547 602 00 Brno Czech Republic	+420 5 4118 2629 +420 5 4118 3152 podborsky@email.cz	IR
Armando Alcaraz	United States of America	Lawrence Livermore National Laboratory University of California Forensic Science Center P.O. Box 808, L-178 Livermore, CA 94551 United States of America	+1 925 423 6889 +1 925 423 9014 Alcaraz1@llnl.gov	GC, IR

[1] An asterisk indicates that the evaluator in question was present at the Twenty-Sixth Meeting of the Group.

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Bedrich Uchytil	Czech Republic	Institute for Protection of Population Laboratory Korunni 2 25168 Kamenice Czech Republic	+420 724 355197 +420 284 685027 bedrich.uchytil@ioolb.izscr.cz	GC, IR

TABLE 2: MS EVALUATORS

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Edward White	United States of America	NIST 100 Bureau Drive Stop 8380 Gaithersburg, MD 20899-8380 United States of America	+1 301 975 3101 +1 301 975 3670 edward.white@nist.gov	**MS Coordinator**
Vesa Häkkinen*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 19150439 +358 9 19150437 vesa.hakkinen@helsinki.fi	MS
Jirí Cermak*	Czech Republic	Research Institute for Organic Syntheses 53218 Pardubice Czech Republic	+420 466 822 351 +420 466 822 978 jiri.cermak@vuos.com	MS
Danian Xu	China	Research Institute of Chemical Defence Laboratory of Analytical Chemistry P.O. Box 1044 102205 Beijing China	+86 10 6976 0259 +86 10 6976 0254 xu600@263.net	MS

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Shigeyuki Hanaoka	Japan	Chemicals Evaluation and Research Institute 1600 Shimo-Takano, Sugito-machi Kitakatsushika-gun Saitama 345-0043 Japan	+81 480 37 2601 +81 480 37 2521 hanaoka-shigeyuki@ceri.jp	MS
Luis Ramalho	Portugal	Instituto Nacional De Engenharia E Tecnologia Industrial (INETI) Estrada Paco Lumiar Lisbon Portugal	+351 21 7165141 +351 21 7168100 luis.ramalho@ineti.pt	MS
Sten-Åke Fredriksson	Sweden	FOI, Swedish Defence Research Agency Div. NBC Defence Cementvagen 20 SE-90182 Umeå Sweden	+46 90 106712 +46 90 106809 sten-ake.fredriksson@foi.se	MS
Mozaffar Eslami	Islamic Republic of Iran	Research Institute of Petroleum Industry (RIPI) P.O. Box 18745-4391 Tehran Islamic Republic of Iran	+98 21 590102<u>1</u> to <u>51</u> (ext. 4817) Direct tel. +98 21 5901092 +98 21 6153397 Eslamim@nioc-ripi.org	MS
Hugh Gregg*	United States of America	Lawrence Livermore National Laboratory, University of California, P.O. Box 808, L-091 Livermore, CA 94551 United States of America	+1 925 423 7501 +1 925 424 2626 Hugh-gregg@llnl.gov	MS
Devendra K. Dubey*	India	Defence R& D Establishment VERTOX Laboratory Jhansi Road Gwalier 474002 India	+91 751 223 3488 +91 751 234 1148 dkdubey@rediffmail.com	MS

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Sally Swindlehurst*	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury, Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 61 3273 +44 1980 61 3830 swilcox@dstl.gov.uk	MS
Marieke van Deursen	Netherlands	TNO Defence, Security and Safety P.O. Box 45 2280 AA Rijswijk Netherlands	+31 15 284 3831 +31 15 284 3963 Marieke.vanDeursen@tno.nl	MS
R. S. Verma*	India	Ministry of Home Affairs Sector 36-A Dakshin Marg, Changigarh-160036 India	+91 172 2615068 +91 172 2605923 rsvermacfslchd@gmail.com	MS
Mehran Babri*	Islamic Republic of Iran	Defence Chemical Research Lab (DCRL), P.O.Box 31585-1461 Karaj, Islamic Republic of Iran	+98-261 2313441 +98-261 2313447 (FAX) dcrl@isiran-net.com	MS

TABLE 3: NMR EVALUATORS

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Lars-Gunnar Hammarström*	Sweden	FOI, Swedish Defence Research Agency Div. Of NBC Defence Cementvagen 20 SE-90182 Umeå Sweden	46 90 106600 46 90 106800 lgham@foi.se	**NMR Coordinator**
Urs Meier*	Switzerland	Spiez Laboratory CH-3700 Spiez Switzerland	+41 33228 1713 +41 33228 1402 urs.meier@babs.admin.ch	NMR

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Harri Koskela*	Finland	VERIFIN P.O.Box 55 00014 University of Helsinki Finland	358 9 19150453 358 9 19150437 harri.t.koskela@helsinki.fi	NMR
Christine Albaret	France	Centre d'Etudes du Bouchet, BP3 91710 Vert le Petit France	33 1 69908421 33 1 64935266	NMR
Ian Holden	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 613770 +44 1980 613822 ihold@dstl.gov.uk	NMR
Robert Maxwell	United States of America	Lawrence Livermore National Laboratory University of California P.O. Box 808, L-255 Livermore, CA 94551 United States of America	1 925 423 4991 1 925 424 2626 Maxwell7@llnl.gov	NMR
Damian Magiera*	Germany	WIS, P.O.Box 1142, 29623 Munster, Germany	+49 5192 136 355 (fax) damianmagiera@bwb.org	NMR

TABLE 4: GC (RI) EVALUATORS

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Martin Söderström*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 19150 438 +358 9 19150 437 martin.soderstrom@helsinki.fi	**GC Coordinator** IR

Name	Country	Address	Phone/Fax/E-Mail	Speciality
Bedrich Uchytil *	Czech Republic	Institute for Protection of Population Laboratory Korunni 2 25168 Kamenice Czech Republic	+420 724 355197 +420-323-673054 bedrich.uchytil@ioolb.izscr.cz	GC, IR
Takeharu Wada*	Japan	Chemicals Evaluation and Research Institute 1600, Shimo-Takano, Sugito-machi Kitakatsushika-gun Saitama 345-0043 Japan	+81 480 37 2601 +81 480 37 2521 wada-takeharu@ceri.jp	GC
Armando Alcaraz*	United States of America	Lawrence Livermore National Laboratory University of California Forensic Science Center P.O. Box 808, L-178 Livermore, CA 94551 United States of America	+1 925 423 6889 +1 925 423 9014 Alcaraz1@llnl.gov	GC, IR

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