Forensic Isotope Ratio Mass Spectrometry Network - Technical Strategy

Dr Susan A Phillips and Sean Doyle

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Forensic Explosives Laboratory,
Dstl Fort Halstead
Sevenoaks
Kent TN14 7BP

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	Name	Signature	
Author	Dr Susan A Phillips		Date
Project Manager	Sean Doyle		Date

Executive Summary

On the 14th May 2003 a Forensic Isotope Ratio Mass Spectrometry (FIRMS) Network Workshop was held at Dstl Fort Halstead. The workshop brought together members of the three working groups that were formed at the FIRMS conference in September 2002.

At the workshop the short, medium and long term research and development objectives were discussed with a view to writing a technical strategy for the FIRMS Network.

This document forms the Technical Strategy for the FIRMS Network. It discusses the short, medium and long-term research and development objectives and discusses the funding opportunities for such research. It is recommended that a review of the current status of research and development into the uses of IRMS in forensic science is undertaken and the review issued to all Network members. A recommendations is also made to the forming of a new Funding Working Group, to assist the technical working groups in obtaining funding for the R&D projects.

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1 Introduction

The Network for Forensic Isotope Ratio Mass Spectrometry (FIRMS) was formed in 2002 by the University of Reading and the Forensic Explosives Laboratory (FEL). The network is funded for three years by the Engineering and Physical Sciences Research council.

The Network aims to raise the awareness of the potential of IRMS in forensic science, crime detection and crime reduction. It also aims to encourage collaboration between chemists, physicists, material scientists and life scientists to stimulate and facilitate the research necessary to meet the scientific objectives.

A conference was held on the 16th and 17th September 2002 which aimed to exchange information between the researchers and end users and to begin to formulate a strategy for the development of IRMS in the field of forensic science [1]. From the conference three working groups were formed:

Explosives Working Group – Sean Doyle (facilitator)
Drugs Working Group – Emma Titterton (facilitator)
General Forensics Working Group – Pam Hamer (facilitator)

On the 14th May 2003 a FIRMS workshop was hosted by the FEL at Dstl Fort Halstead. The working groups were asked to consider a number of points that would be used to produce the technical strategy. From the workshop a list of short, medium and long term research and development objectives were produced [2].

This document aims to outline a strategy for how the FIRMS Network will develop IRMS in the field of forensic science.

2 Network Membership

It was an objective of the original proposal that the network bring together IRMS researchers, end users and instrument manufacturers. End users may include forensic scientists, police officers and those in the legal profession.

The network has been supported, to date, by members of each of these communities. However, expansion of the network membership should be encouraged. This will include those who may only want to keep a watching brief on developments in the field to those who want an active participation in the network.

To encourage membership effort should be made to publicise the network at suitable fora. This may take the form of oral or poster presentations. Promotion should be made not only in the field of forensic science but also in the legal and police forums and in non-forensic scientific fields that use IRMS.

Forums for publication of the network should be identified and attended by network members.

3 Target materials and applications

3.1 Priority target materials

It was recognised at the FIRMS Workshop that to secure funding for forensic IRMS development demand for the technique needs to justify the maintenance of such a capability. The technique will therefore need to apply primarily to high volume and high value crime. In addition to prioritised target materials, consideration needs to be given to the target elements.

It is recognised that different laboratories in different countries may have different priority materials. Effort will be given to choosing materials common or beneficial to all laboratories.

3.1.1 Explosives

When agreeing the list of priority explosives to be studied consideration must be given to the current explosive threats. Organic explosives may be recovered in a 'pure' form, e.g. TATP, TNT, or may be contained within an explosive formulation, e.g. PE4. Inorganic explosives normally comprise a mixture of inorganic oxidisers and fuels, e.g. sugar/chlorate, flash powder. Priority explosives are suggested as being:

- Organic high explosives e.g. RDX, PETN, TNT, NG (^{13}C, ^{15}N, ^{18}O)
- Smokeless powders (^{13}C, ^{15}N, ^{18}O)
- Inorganic nitrates e.g. ammonium nitrate, potassium nitrate (^{15}N, ^{18}O)
- Peroxide explosives TATP (^{13}C, ^{18}O) and HMTD (^{13}C, ^{15}N, ^{18}O)
- Sodium chlorate, sodium perchlorate (^{35}Cl)
- Accelerants (^{13}C)

Ongoing evaluation of forensic explosive threats may give rise to new priority explosives.

3.1.2 Drugs

The list of priority drugs may include both pharmaceutical formulations and illicit drugs e.g. ecstasy, heroin. It was agreed at the FIRMS workshop that the priority drugs are:

- Amphetamines (^{13}C, ^{15}N)
- Heroin (^{13}C, ^{15}N)
- Cocaine (^{13}C, ^{15}N)

3.1.3 General Forensics

There is a wide range of materials other than drugs and explosives for which it would be useful to determine the isotopic ratios for crime detection e.g. glass, paint, inks. When choosing materials for the priority list it is useful to choose materials that would be encountered in a wide variety of high volume or value crimes. The priority list will include:

- Packaging materials (^{13}C, ^{2}H)

3.2 Target applications

There are three main target applications:

3.2.1 Forensic comparison of bulk samples

This is the simplest application for IRMS is the field of forensic science. The isotope ratio values for elements in the bulk samples can be compared to determine whether the samples may have originated from the same source. If the isotope ratios of the two samples are significantly different then it may be concluded that the samples did not originate from the same source. Problems with interpretation arise when the isotopic values are similar or identical. Knowledge of the within batch heterogeneity and the likelihood of products from the same source having the same isotopic values is required to make this interpretation. This requires knowledge of the synthesis or manufacturing processes. It has been generally found that the use of more than one isotope increases the discrimination power of the technique.

The simplest form of bulk analysis is to characterise the material as a whole, i.e. PE4 rather than to extract the sample into its constituent's e.g. RDX, binders, waxes. However, greater discrimination between samples may be achieved by analysing the individual components. This may be achieved through the use of an off-line sample preparation techniques e.g. liquid/liquid extraction, preparative HPLC, or through an on-line compound specific technique such as GC-C-IRMS.

3.2.2 Forensic comparison of trace materials to a bulk or other trace.

The next stage for IRMS is in the application to trace samples. This will require on-line compound specific IRMS techniques. The processing of trace samples normally involves a recovery technique, such as swabbing, an extraction technique and a cleanup technique. Studies will be required to determine that the isotopic signatures of the original material are preserved through the deposition, recovery, extraction and cleanup processes.

Explosives trace analysis can be applied to pre-explosion traces and post-explosion traces. Studies will be required to determine whether or not the isotopic signature is preserved through the explosion.

3.2.3 Determination of the origin of bulk or trace materials.

This is the most complex use of IRMS and will require databases of the isotopic ratio values of target materials from different suppliers around the world. The population of such databases will be an enormous undertaking.

3.2.4 Other forensic applications of IRMS

The full potential of IRMS in the field of forensic science will only be realised as the project progresses. Other potential applications are listed below:

- Prediction of the isotopic signature of a product from knowledge of the signatures of the starting material (to link, for example, an improvised explosive found in a device to starting materials found at a suspects house).

- Identification of human movement from knowledge of the turnover of elements in the body.

4 Short, Medium and Long Term Research and Development Objectives

The scientific objectives of the Network are to:

- Identify the range and extent of heterogeneity of isotopic compositions of manufactured materials and determination of the factors that govern these values.
- Examine how isotopic compositions change during and after manufacture.
- Identify the range of compounds to which this technique applies.
- Extend the scope of IRMS beyond the current work in drugs and explosives.
- Define the limitations of the technique.

Prior to formulation of proposals to cover the short, medium and long-term objectives a review of the current status of research and development into the use of IRMS in the field of forensic science should be undertaken. This review should identify past research, current research and the duration and scope of current programmes. Much can be learned from other scientific disciplines with well-established experience of IRMS i.e. geochemistry.

4.1 Short Term Objectives

The short-term objectives are those that are achievable within the next three years. To secure funding initially the requirement will need to concentrate on high volume and high value crime. The short-term objectives will be applied to the priority applications and target materials. Techniques will be developed and validated to allow for the forensic comparison of bulk materials. Thought will be given to the requirements for databases.

- Agreement and validation of reference materials and working standards.
- Research and development of validated standard methods or standardised results for the target materials at bulk level.
- Preliminary investigation of batch variation during the synthesis or manufacture of commercial and improvised materials.
- Investigation of the effect of packaging/storage on the preservation of isotopic ratios of bulk target materials/elements.
- Databases – preliminary study into requirements, structure, custody and population.

4.2 Medium Term Objectives

The medium term objectives, i.e. those achievable within three to five years, will assume that validated standard methods or methods that produce standardised results are

available for all the priority target materials. In this timescale off-line techniques for compound specific analysis of bulk materials will be developed and validated. Preliminary investigations into on-line compound specific techniques for trace analysis will be undertaken. Population of the databases will be underway.

Aim: To undertake research and development to allow compound specific analysis and the forensic comparison of trace and bulk materials.

- Compound specific IRMS – using off-line techniques, investigation of isotopic fractionation during the preparative process.
- Preliminary investigation into trace techniques.
- Continuation of batch variation studies.
- Population of databases.
- Review of the technical strategy and long term objectives.

4.3 Long Term Objectives

The long-term objectives are those achievable within five to ten years. Within this time scale it is envisaged that techniques and studies into trace analysis using on-line compound specific techniques will be fully developed. Databases allowing determination of the global origin of a material will be in an advanced state. Research will focus on high throughput screening of samples and broadening the scope to other materials and applications.

- On-line compound specific IRMS – development of analytical techniques and investigation of isotopic fractionation.
- Trace analysis – including the effect of sample deposition, recovery, extraction and cleanup techniques on the preservation of isotopic ratios.
- Determination of the origin of traces and bulk materials.
- High sample throughput.
- Population of databases.
- Broadening the scope to other materials.
- Broadening the scope to heavy elements, through the use of, for example, ICP-MS.

5 Funding

It has been recognised that to secure funding initially for forensic IRMS development the scope should cover high volume and high value crime. A number of different funding pathways have been identified.

Laboratories may already have current programmes of work related to forensic IRMS, the results of which may be available to other network members. Laboratories may be able to apply for funding within their own organisation or Government, with or without collaboration from external laboratories. These types of funding may enable other laboratories to act as contractors or sub-contractors. There is the potential for joint research proposals to be submitted to national or international funding bodies.

5.1 UK Science and Engineering Research Councils

The FIRMS network is funded by the Engineering and Physical Sciences Research Council. The UK research councils are potential sources of funding. Applications need to be submitted by academic organisations, but support from the end users i.e. forensic laboratories or the police, is often a requirement of the proposal.

There is the possibility of research and development work being undertaken as PhD studentships, with funding from the UK research councils and organisations such as the Royal Society of Chemistry. Some financial contribution is normally required from the supporting organisation. This route offers an inexpensive means by which research and development into the longer-term objectives may be carried out.

5.2 UK Home Office

The Forensic Explosives Laboratory (FEL), Forensic Science Service (FSS) and Police Scientific Development Branch (PSDB) are able to bid into the Home Office Science Policy Unit research and development funds. This is done on an annual basis, funding commencing in April of each year. The FEL, FSS and PSDB are able to use other laboratories as contractors.

5.3 European Union Funding

The European Union 6th Framework programme covers activities in the field of research, technological development and demonstration for the period 2002 to 2006. The Framework programme does not cover all areas of science and technology, rather a limited number of thematic priorities have been identified. In general, the EU contributes only a certain percentage of the total costs of a project. Only consortia of partners from different member and associated countries can apply, with one of the project participants acting as co-ordinator.

5.4 International Funding

Other countries will have their own scientific research councils and sources for Government funding. For example, there are a number of potential funding opportunities from within the US e.g. Technical Support Working Group (TSWG), National Institute of Justice. These proposals will normally need to be led by organisations from within that country.

5.5 Mechanism for funding

Application for funding can be a time consuming process. It is recommended that a Funding Working Group be formed to focus the effort for funding application. The Funding Working Group should comprise representatives from the UK, EU, US, Australia and New Zealand. Those representatives should cover both academic funding and government funding. The funding working group would assist the scientific working groups to obtain funding in their relevant country. It is recommended that a review of funding sources in the Network countries be undertaken.

6 Recommendations

There are a number of tasks that can and should be undertaken prior to the formulation of proposals to cover the research and development objectives.

- Fora for publication of the network should be identified and attended by network members.

- Formation of a Funding Working Group, to assist the scientific working groups with applications for funding. The group should ideally contain members of each country represented in the Network and should comprise personnel able to assist with the different types of funding i.e. academia, Government. Initially the Funding Working Group should review all potential funding bodies/organisations and obtain details of the application requirements, deadlines etc. This document should be issued to all network members.

- Review of the current status of research and development into the use of IRMS in forensic science, including identification of past research, current research, duration and scope of current programmes. The review should be issued to all Network members.

- Identification of FIRMS Network members able to undertake experimental work.

7 Acknowledgements

The authors wish to thank the Network members for their continued support and the Engineering and Physical Sciences Research Council for funding.

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FIRMS Network Members

2. Jose Almirall, Director Forensic Science Graduate Program, Department of Chemistry, Florida International University, U.P. 11200 SW 8th Street, Miami, Florida 33199 USA.

3. Mark Bailey, Centre for Ecology and Hydrology, IVEM, Mansfield Road, Oxford OX1 3SR.

4. Stephen Barrett, Dstl, Winfrith Technology Centre, Dorchester, Dorset, DT2 8WX.

5. Johannes Barth, SUERC, Rankine Avenue, East Kilbride, Glasgow, G75 0QF.

6. Tom Bassindale, Drug Control Centre, Kings College London, 150 Stamford Street, London, SE1 9NN.

7. John Bellerby, DEOS, Cranfield University, RMCS Shrivenham, Swindon, SN6 8LA.

8. Sarah Benson, Australian Federal Police Services, GPO Box 401, Canberra ACT, Australia.

9. David Carter, LGC Ltd, Queens Road, Teddington, Middlesex, TW11 0LY.

10. James Carter, Organic and Biological Section, School of Chemistry, University of Bristol, Cantocks Close, Bristol BS8 1TS.

11. Thure Cerling, Dept Geology, 135 South 1460 East, University of Utah, Salt Lake City, Utah 84112, USA.

12. Max Coleman, PRIS, University of Reading, Whiteknights, Reading RG6 6AB.

13. Tyler Coplen, US Geological Survey, 431 National Centre, Reston, VA 21092, US.

14. Lorna Corr, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS.

15. Stewart Craig, ThermoFinnigan Ltd, 576 Chester Road, Sandiway, Northwich, CW8 2DU.

16. Debra Croft, FGU (Geology), Queens Royal Holloway, Egham, Surrey TW20 0EX.

17. Gareth Davies, Faculty of Earth and Life Sciences, Vrije Universiteit, De Bolelaan 1085, 1081 HV Amsterdam, The Netherlands.

18. Mary Donohue, Managing Director ISEF, 20 Wyndemere Road, Broomfield, CT 06002, USA.

19. James Ehleringer, Dept Biology, University of Utah, 257 South 1400 East, Salt Lake City, Utah 84112, USA.

20. Ben Fairman, LGC Ltd, Queens Road, Teddington, Middlesex, TW11 0LY.

21. Hilmar Foerstal, Forschungszentrum Julich, ICG IV, 52425 Julich, Germany.

22. Francois Fourel, Micromass UK Ltd, Floats Road, Wythenshawe, Manchester, M23 9LZ.

23. Russell Frew, Dept Chemistry, University of Otago, PO Box 56, Dunedin, 9001, New Zealand.

24. Gardebas, Institut de Recherche Criminelle de la Gendarmerie Nationale, 1 Boulevard Theophile Sueur, Rosny-sous-Bois, France.

25. Pam Hamer, Forensic Alliance Ltd, F5 Culham Science Centre, Abingdon, Oxfordshire, OX14 3ED.

26. Tom Hannigan, Forensic Science Laboratory, Garda Headquarters, Phoenix Park, Dublin 8, Republic of Ireland.

27. Shabana Haque, PSDB, Sandridge, St.Albans, Hertfordshire, AL4 9HQ.

28. Jeffrey Heikoop, Hydrology, Geochemistry and Geology Group, Earth and Environmental Sciences Division, Mailstop D462, Los Alamos, New Mexico 87545, USA.

29. Jurian Hoogewerff, Mass Spectrometry Team, Institute of Food Research, Norwich Research Park, Colney, Norwich, NR4 7UA.

30. John Howa, University of Utah, 354 South 1300 East, Salt Lake City, Utah, 84103 USA.

31. John Jasper, Molecular Isotope Technologies, 8 Old Oak Lane, Niantic, Connecticut 06357-1815, USA.

32. Sue Jickells, Forensic Science Unit, School of Health and Life Science, Kings College London, Franklin-Wilkins Bldg, 150 Stamford St, London SE1 9NN.

33. Julianna Fessendon, Earth and Environmental Sciences Division, Hydrology, Geochemistry and Geology Group, EES-6, MS-D462, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA.

34. Pier de Groot, Pastoor Moorkensstraat 16, 2400 Mol – Achterbos, Belgium.

35. Robert Kalin, Queens University Belfast, School of Civil Engineering, David Keir Bldg, Stranmillis Road, Belfast, N.Ireland BT9 5AG.

36. George Kee, Forensic Science Northern Ireland, Seapark, 151 Belfast Road, Carrickfergus, N.Ireland BT83 8PL.

37. Carol Kendall, US Geological Survey, 345 Middlefield Road, MS 434, Menlo Park, California 94025, USA.

38. Simon Kelly, School of Environmental Science, University of East Anglia, Norwich, NR4 7TJ.

39. Helen Kreuzer-Martin, Dept Biology, 257 South 1400 east, University of Utah, Salt Lake City, Utah 84112-0840 USA.

40. Steven Krueger, FBI Academy, Quantico, VA, USA.

41. John Lanham, Stable Light Isotope Unit, Archaeology Department, University of Cape Town, Private Bag Rondebosch 7700, South Africa.

42. Andrew Linton, PDZ Europa Ltd, Langdale House, Gadbrook Business Centre, Rudheath, Northwich, Cheshire, CW9 7TN.

43. Janice Lofthouse, Central Science Laboratory, Sand Hutton, York YO41 1LZ.

44. Michael Lott, Dept Biology, University of Utah, 257 South 1400 East, Salt Lake City, Utah 84112-0820 USA.

45. Arnaud Maitre, Institut Universitaire de Medecine Legale, Laboratoire Suisse d'Analyse du Dopage, Rue du Bugnon 21, 1005 Lausanne, Switzerland.

46. Sandro Meli, Dip. Scienze della Terra, Universita di Parma, Parco Area delle Scienze 157/a, 43100 Parma, Italy.

47. Nikolaas van der Merwe, Archaeology Department, University of Cape Town, Rondesbosch 7701, South Africa.

48. William Motzer, Todd Engineers, 2200 Powell Street, Suite 225, Emeryville, California 94608, USA.

49. Anna Mukherjee, Organic Geochemistry Unit, School of Chemistry, University of Bristol, Cantocks Close, Bristol BS8 1TS.

50. Norbet Naulet, LAIEM, University of Nantes, 2 ruw de la Houssiniere, 44322 Nantes, Cedex 3, France.

51. Wendy Norman, RCMP Forensic Laboratory Services, 1200 Vanier Parkway, PO Box 8885, Ottawa, Ontario K1G 3MB, Canada.

52. Fabien Palhol, Laboratoire des Dovanes de Paris, 1 Rue G Vicaire, Paris 75003, France.

53. Angelika Preiss-Weigert, BgVV Thielalle 88-92 Postfach 33 00 13 D-14191, Berlin, Germany.

54. Tom Preston, SUERC, University of Glasgow, Rankine Avenue, East Kilbride, G75 0QF.

55. Steve Price, Pelican Scientific Ltd, Chester Road, Aldford, Chester CH3 6HJ.

56. Clemente Recio, Stable Isotope Laboratory, Facultad de Ciencias, University de Salamanca, Plaza de la Merced, S/N E 37008, Salamanca, Spain.

57. Sam Blittman, Arson Laboratory Consultants, 2864 Wildflower Drive, Antioch, California 94531-6360, USA.

58. Karyne Rogers, Stable Isotope Laboratory, Rafter Building, Institute of Geological and Nuclear Sciences Ltd, PO Box 31 312, Lower Hutt, New Zealand.

59. William Showers, Dept MEAS, Box 8202, North Carolina State University, Raleigh, North Carolina 27695, USA.

60. George Stewart, Faculty of Life and Physical Sciences, University of Western Australia, Crawley 6009, Western Australia.

61. Richard Strobel, ATF Forensic Science Laboratory, 1401 Research Blvd, Rockville, MD 20850, USA.

62. Emma Titterton, Mass Spec Analytical Ltd, Building 20F, Golf Lane, Filton, Bristol BS99 7AR.

63. Thomas Tutken, Institut fur Geowissenschaften, Universitat Tubingen, Wilhelmstrasse 56, D-72074, Tubingen, Germany.

64. David Tranthim-Fryer, Chemistry Centre (Forensic Science Laboratory), 125 Hay Street, East Perth, WA 6004, Australia.

65. Shaun Tumelty, Northumbria Police, Scientific Support, Headquarters, Ponteland, Newcastle upon Tyne, NE20 0BL.

66. Gerard van der Peijl, Netherlands Forensic Institute, PO Box 3110, 2280 GC Rijswijk, The Netherlands.

67. Mike Verkouteren, Mailstop 8372, National Institute of Standards and Technology, Gaithersburg, Maryland 20899 USA.

68. Robert Vocke, NIST Analytical Chemistry Division, 100 Bureau Drive, Gaithersburg, Maryland 20899-8391, USA.

69. Ruth Waddell, Mailstop K484, Los Alamos, New Mexico 87545, USA.

70. Darcos Wattimena, JLD Wattimena Erasmus MC, Dept of Internal Medicine, PO Box 2040 3000 CA, Rotterdam, The Netherlands.

71. Rowan White, Analytical Precision Products Ltd, Windsor House, Gadbrook Park, Northwich, Cheshire CW9 7TN.

72. Larissa Wolf, Netherlands Forensic Institute, PO Box 3110, Rijswijk, Netherlands, NL-2280 GC.

73. Wolfram Meier-Augenstein, University of Dundee, School of Life Sciences, Old Medical School, Dundee, DD1 4HN.

74. Stephan Woodborne, QUADRU, Environmentek, Box 395, Pretoria 0001, South Africa.

75. Kimberly Young, Forensic Science Service, Trident Court, Solihull Parkway, Birmingham Business Park, Solihull B37 7YN.

Non-Dstl

76. Graham McAlister, Home Office TPU, 50 Queen Anne's Gate, London SW1 9AT.

77. DCI Keith Pearce, Metropolitan Police SO13, New Scotland Yard, Broadway, London SW1H 0BG.

78. Staff Officer to the Chair of ACPO(TAM), Metropolitan Police, New Scotland Yard, Broadway, London SW1H 0BG.

79. Staff Officer to the Secretary ACPO(TAM), Metropolitan Police, New Scotland Yard, Broadway, London SW1H 0BG.

80. ACPO(TAM) R&D, Mr Colin Smith ACC SO, Hampshire Police HQ

81. Keith Asman, Metropolitan Police SO13 Exhibits Office, New Scotland Yard, Broadway, London SW1H 0BG.

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82. TCL (SP)

83. DM ETD

84. TC/ETD

85. Maurice Marshall, Hd/FEL

86. Sean Doyle, Hd Chemistry and Research FEL

87. Cliff Todd, Principal Forensic Investigator, FEL

88. Susan A Phillips, FEL

89. Knowledge Services, Kentigern House, Glasgow, G2 8EX

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