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Forensic Isotope Ratio Mass Spectrometry Network

FIRMS Guidance for the Forensic Interpretation of Isotope Ratio Data

Isotope Ratio Mass Spectrometry

First Edition 2020

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Preface to the first edition

This guidance document for the interpretation of isotope ratio data has had a long and at times difficult gestation. Drawing together the experiences of institutional members of the FIRMS Network working as forensic practitioners applying isotope ratio analysis within various jurisdictions worldwide into single, generally applicable guidance document has been no mean feat. Both Sean Doyle and Gerard van der Peijl have worked tirelessly drafting, revising, and editing countless earlier versions – some quite different to this! - and I thank both of them together with the other members of the FIRMS Network who have contributed in one way or another to this document for producing such a valuable resource to the forensic isotope ratio community.

As with the Good Practice Guide for Isotope Ratio Mass Spectrometry, this document is aimed at providing both experienced forensic practitioners and relative newcomers a helping hand, this time when interpreting rather than obtaining their isotope ratio data in a forensic context.

Interpretation is undoubtedly a complex subject which we have tried to simplify in this guide. The FIRMS Network welcomes any and all feedback, whether complimentary or critical so that future editions of this guidance can be improved.

Dr Phil Dunn

Chair (2015-present) and Director

The FIRMS Network

Disclaimer

Reference to or mention of any commercial product or process by specific trademark or manufacturer within this guide does not represent a recommendation or an endorsement by the FIRMS Network, nor does it imply that any of the materials, instruments or equipment identified are necessarily the best available for the purpose described.

Feedback

If you have any comments about this guide, suggestions for improvement or ideas for topics that should be included in future editions please let us know at:

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Thank you.

Contents

1 Introduction

This Guide sets out good practice in the interpretation of isotope ratio data in the context of an enquiry conducted by a judicial, regulatory, or other tribunal. Compliance with this Interpretation Guide, together with the latest edition of the FIRMS Good Practice Guide [Dunn and Carter 2018], will assist such tribunals to reach a safe decision by a fair process.

The guidance on interpretation offered in Section 8 of the Good Practice Guide should be taken in conjunction with that offered in this Guide. Together they represent good practice as recommended by the FIRMS Network.

This Guide aims to be of practical use and therefore the more complex aspects of the interpretational process are avoided. Readers wishing to learn more or delve more deeply should study the documents referred to in this Guide. A standard text on the subject is Robertson, et al. [2016]

2 Terms & definitions

The terms are defined in the order in which they appear in the text. Only those terms that might be unfamiliar to the reader are included.

Term	Description
Tribunal	Any institution or person with the authority to adjudicate in legal, regulatory or other disputes. Its purpose in settling claims and disputes is to establish facts.
Source	The origin of an evidential material which may be, but is not limited to, geographical provenance, manufacturer, batch, starting material, synthetic route, or biochemical pathway.
Evidential strength	The degree to which evidence supports one of a pair of mutually exclusive propositions under consideration by a tribunal. It is similar in meaning to evidential or probative value.
Likelihood ratio	A ratio of conditional probabilities, the value of which is a measure of the degree of support for one of a pair of mutually exclusive propositions under consideration by a tribunal.
Fact finder	That part of the tribunal with the duty to decide questions of fact. In legal tribunals the fact finder is the jury or judge. In regulatory or other tribunals, the tribunal itself may be the fact finder.

3 Forensic utility

Isotope ratio analysis is employed for source inference. However, its limitations are recognised [Gentile et al. 2015, Cerling et al. 2016]. These limitations are such that isotope ratio data alone are unlikely to be sufficient to resolve the question of source. Besides having a sufficient background dataset, isotope ratio data will often be employed in conjunction with complementary techniques. That being recognised, there are circumstances in which isotope ratio data can be particularly useful in addressing the question of source, particularly where chemical composition sheds little light.

It follows that, in addition to interpreting isotope ratio data, expertise in the interpretation of data generated by complementary techniques will also be required. That expertise need not necessarily be possessed by/reside in one and the same person

4 Scope

This guide applies to service providers which interpret isotope ratio data in the context of a particular enquiry for the purpose of source attribution of one type or another. The analyst acquiring the data using the appropriate scientific instruments does not necessarily have to be the person doing the interpretation, provided enough information is available to the interpreter regarding the collection of the data. Conversely, if the service provider solely provides isotope ratio data with no interpretation, then this guide does not apply.

The process of interpretation set out in this guide is one that arrives at a so-called evaluative opinion, that is an opinion of evidential strength[1]. Fundamental to this approach is the consideration of alternative, mutually exclusive hypotheses or propositions and an assessment of the probability of the evidence given those hypotheses. Other interpretational processes fall outside the scope of this guide.

[1] Some authors use the term 'weight' which is acceptable as it is a term that has a legal meaning. However, weight is strictly log10 of the likelihood ratio [2].

5 Requirements

5.1 Methods

Methods used to generate isotope ratio data for interpretation must conform to recommendations of the current edition of the FIRMS Good Practice Guide [Dunn and Carter 2018] to the fullest extent achievable, take account of the requirements set out in Dunn et. al. [2017], and preferably should be accredited to the International Standard ISO/IEC 17025:2017. Where the method is not accredited then validation must have included interlaboratory comparison as a means of demonstrating comparability of measurement.

Metrological traceability to internationally agreed reporting scales is essential and measurement uncertainty must be evaluated. The result is not complete and cannot be properly interpreted unless it is accompanied by a quantitative statement of its uncertainty as well as a coverage factor if it is expressed as expanded uncertainty.

The preparative, instrument, and data handling methods selected will depend on the type of material(s) and source in question. They should meet the needs of all stakeholders, in particular those of the parties to the tribunal and the pertaining judicial or regulatory system.

5.2 Logical Interpretation

The interpretation of isotope ratio data along with other complementary data in the context of a particular enquiry should, to the fullest extent achievable, conform to the standards set out in the AFSP Standard [Doyle and Doyle 2012, AFSP 2009] and ENFSI Guide [Champod et al. 2016]. These Standards are based on four fundamental requirements.

(1)	Balance	Alternative, mutually exclusive hypotheses are always considered
(2)	Logic	The probability of the data given the hypothesis is considered and not the probability of the hypothesis given the data
(3)	Robustness[2]	Data are generated by validated, preferably accredited methods employed by competent operators
(4)	Transparency	The process of interpretation is made clear

The process set out in these Standards involves the assignment of a likelihood ratio (*LR*) as a measure of the strength of evidence in support of a common source. Regardless of whether the *LR* is assigned based on subjective or empirical information, or both; as a minimum a verbal statement of strength should be reported; examples are appended as Table 1.

In the context of a criminal investigation, the convention is that an $LR < 1$ strengthens the defence case and/or weakens the prosecution case, while an *LR* close to unity renders the evidence irrelevant and strictly inadmissible. An $LR > 1$ strengthens the prosecution case. Scales exist for expressing degrees of support, in the case of $LR \approx 1$ equal support for both hypotheses, with increasing values of the *LR* providing a greater degree of support.

A practical example of the process is as follows. The question is; are the illicit materials from the same batch? The prosecution proposition or hypothesis is:

H_P - the illicit materials are from the same batch

And the defence hypothesis is:

H_D - the materials are not from the same batch

The *LR* is assigned by considering the probability of the degree of resemblance between the data (the evidence *E*) given that the materials are from the same batch $p(E|H_P)$ and the probability of the evidence given that the materials are not from the same batch $p(E|H_D)$.

[2] Compliance with the FIRMS Good Practice Guide will support the requirement for robustness.

The likelihood ratio is obtained by ratioing these conditional probabilities (1).

$$LR = \frac{p(E|H_P)}{p(E|H_D)} \quad (1)$$

Clearly, the investigators need background data sufficient in quantity, quality, and relevance to establish these probabilities; examples include inter- and intra-batch variation in materials of the same type as the evidence.

If the assigned *LR* is close to 1, the evidence provides equal support for both the defence and prosecution's hypothesis and therefore is irrelevant. If the *LR* is > 1 then, to some degree, the evidence is more supportive of the prosecution's hypothesis of the same batch. As the *LR* increases in value from 1, the scale can be verbally translated from; no support to weak, moderate, strong, and very strong support. In this example, the probability of the evidence is greater if the prosecution hypothesis is true rather than the defence hypothesis and the assigned *LR* equates to strong support for the hypothesis that theillicit materials are from the same batch.

In addition to reporting the strength of evidence, the scale must also be reported together with a description of the process of interpretation. This satisfies the requirement for transparency.

There is in fact a hierarchy of propositions from which hypotheses are derived. The members of the hierarchy are: offence, activity, and source. In most circumstances the offence level is addressed by the fact finder. The other applicable level is 'activity,', including the probability of transmission or non-transmission of trace evidence. The ENFSI Guide recommends evaluation at/consideration of activity level wherever possible and that indeed is good practice. However, as isotope ratio data is usually employed to address only source level propositions, the consideration of activity level propositions falls outside the scope of this Guide.

To be clear, the propositions considered based on isotope ratio data alone will relate to whether evidential materials are from the same source, which could be defined as:

- geographical region,
- manufacturer,
- batch and/or lot,
- starting materials,
- synthetic route, and/or
- biochemical pathway.

The definition of the source and the relevance and availability of background data must be defined early in the process and clearly stated.

5.3 Factors affecting interpretation

Depending on the type of source in question, one or more of the following potentially confounding factors need to be considered:

- manufacturing process,
- background source level variation,
- temporal variation,
- homogeneity,
- stability,
- sample integrity.

The manufacturing process will vary within controlled industrial scale production, where inter- and intra-batch variation, changes in the production parameters, and changes in raw materials are all potentially confounding factors. In small-scale manufacture, such as synthesis of illicit substances,

the process may be less controlled, providing greater isotope ratio variation between small batch sizes.

While all are important, the most challenging aspect of addressing source-level propositions will be gaining reliable data to determine the background source level variation. This may involve the creation of a database of material from a sample of a relevant population, e.g. tissue, plastic adhesive tape, cable ties, plastic cord/rope, plastic bags, reactants and products, each from a relevant source. For the reliable comparison of isotope data between evidence and background data, traceability and comparability of measurement are essential.

In investigations of diet and provenance (e.g., for materials from human, wildlife, livestock, food, water, and other sources) suitable databases may already exist. However, the requirements of measurement traceability and comparability must still be satisfied.

The relevance of the database to the enquiry, i.e. its fitness-for-purpose, must be made clear to satisfy the requirement for transparency. For example, a database of isotope ratios of ancient ivory samples may not be appropriate for evaluation of ivory evidence collected from recently deceased animals.

In order to assure the relevance of the database it may be necessary to obtain some case-specific information. Such a step may increase the risk of cognitive bias[3] affecting the interpretation. However, focussing on the strength of the evidence given two competing hypotheses, and not the probability of the hypothesis, will reduce the likelihood and the potential impact of any such bias. In addition, due to the numerical, continuous data provided by isotope ratio analysis, the interpretation of data should be less subjective than many other evidence types and, as a result, less prone to cognitive bias.

5.4 Peer review

The process of interpretation must include peer review by an equally qualified individual, preferably blinded to the original conclusion and irrelevant circumstantial detail. A procedure must be in place to resolve any differences between the reviewer and the reporting scientist.

5.5 Legal Obligations

Judicial and regulatory systems may vary but the standard of scientific evidence should not. Scientific evidence must be reliable to the extent of assisting a tribunal to reach a safe decision by a fair process. This is best achieved by following the practice set out in the FIRMS Good Practice Guide and in this Interpretation Guide.

The legal obligations of a forensic scientist acting as an expert witness are generally accepted to be as follows:

- not to usurp the role of the fact finder,
- duty is to the tribunal and not the instructing/commissioning party,
- provide evidence that is independent, impartial, unbiased, and objective,
- provide evidence within field of expertise,
- set out the reasons for the opinion/conclusion,
- provide details of any tests carried out by others which are relied upon, and
- state and clearly explain any limitations.

These obligations must be discharged. One certain means of doing so in relation to some of those obligations is to restrict interpretation to the assignment of an *LR* and report the strength of the

[3] Guidance on reducing the risk of cognitive bias is available from the Office of the Forensic Science Regulator.

evidence verbally rather than numerically. However, avoiding usurping the role of the fact finder can be difficult.

Offering a categorical opinion of the type match/uncertain/non-match must rely on information which is properly the province of the fact finder. Indeed, the opinion itself is one for the fact finder and not for the expert witness who, in offering such an opinion, has considered the probability of the hypothesis given the evidence.

How the fact finder's role might be usurped is most easily explained by considering Bayesian inference in general, in which prior beliefs are updated in the light of new information.

$$\text{Current beliefs} = \text{Prior beliefs updated by the } LR \qquad (2)$$

This corresponds to the tribunal process whereby the fact finder in a criminal trial considers the probability of guilt given the evidence. The fact finder's belief is updated by the evidence provided by the expert witness who reports only that the probability of the evidence is greater given one hypothesis rather than an alternative. The fact finder then updates its belief arriving at the current belief.

In terms of a criminal trial, a practical example might be as follows. The expert reports that the degree of resemblance found between the isotopic signatures of the ligature used to tie the victim and that of the roll of twine associated with a suspect is far more likely given that they are from the same source rather than from random different sources. If such evidence is supportive of the prosecution case – and in this example, it is – then the jury updates its prior belief and arrives at a current belief in which the probability of guilt has increased.

In determining whether the role of the fact finder has been usurped, a simple test is to determine whether the probability of the evidence given the hypothesis ($pE|H$) is being provided by the expert witness. If it is, then the duties of an expert witness are being discharged properly. If the probability of the hypothesis given the evidence ($pH|E$) is being provided by the expert witness, then the role of the fact finder has been usurped and, as a result, the evidence is misleading.

Other duties that should be considered include not burdening the tribunal with evidence that is not germane to the matter in dispute, and not presenting misleading evidence. If data will not assist the tribunal or may mislead it then the evidence must not be adduced. Opinions of the type '… *consistent with* …' are misleading and '… *cannot exclude* …' can be misleading. Again, the way of avoiding these issues is to interpret the evidence as set out in this Guide.

6 Summary

This Interpretation Guide sets out the scientific, quality, and legal requirements that should be met when interpreting isotope ratio data in the context of a particular enquiry. The quality of the data is assured by complying with the current edition of FIRMS Good Practice Guide and accreditation, or at least full validation, of the method employed. Metrological traceability is essential and measurement uncertainty must be evaluated. The fundamental interpretational requirements are balance, logic, robustness, and transparency. The interpretation of isotope ratio data is usually limited to the consideration of source level propositions where the probability of the evidence given two mutually exclusive hypotheses is considered and a likelihood ratio assigned, thereby evaluating the strength of the evidence. When reporting the strength of evidence, the scale from which the degree of support is selected must also be reported. A number of potentially confounding factors must be taken into account when interpreting IRMS data. Background data must exist where the quality and reliability of the populating data must be assured and its fitness-for-purpose clearly established. The Guide sets out the legal obligations that must be met. Compliance with this Guide assures good practice in interpreting isotope ratio data and assisting tribunals, of whatever type, to reach a safe decision by a fair process

***Table 1**. Example verbal statements of evidential strength*

LR	**Verbal Statements**		**In a criminal trial**
<1	Evidence is more likely if the alternative proposition is true	Provides (degree of) support for the alternative proposition	Evidence strengthens the defence case
≈1	Evidence is equally likely given either proposition	Supports neither proposition	Evidence is irrelevant
>1	Evidence is more likely given the proposition	Provides (degree of) support for the proposition	Evidence strengthens the prosecution case

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