

Letters to the Editor

Central Research Establishment: Reports

Sir:

I would be most grateful if you would bring to the attention of contributors to the *Journal of Forensic Sciences* that the above report series is for internal use only and should be cited as personal communications in the published literature. As you will appreciate, publications from an establishment such as ours are subject to strict editorial procedures. However, in an effort to speed up the dissemination of our work, we have made our internal reports available on limited circulation. These reports have not been passed through the usual procedures, hence our reluctance to see them cited freely.

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Discussion of "Microcomputers in Forensic Science"

Dear Sir:

The article "Microcomputers in Forensic Science" by Neiburger (Vol. 30, No. 3, July 1985, pp. 881-892) in the *journal* contains one point that may be a bit misleading to those unfamiliar with several different microcomputers. In discussing communication programs (p. 889), the author states "Different brands of computers can exchange data over the modem. Records, files, graphics and raw numeric data can be quickly telephoned around the world." While it is true that data files which have been stored in a standard American Standard Code for Information Interchange (ASCII) format can be interchanged between different brands of computers, this is not generally true of graphics. Because of differences in hardware, screen memory, mapping, and resolution, graphic codes are not standardized and differ widely from one computer to the next, even among products from the same manufacturer. Thus, graphics containing files or programs cannot be readily interchanged. In some instances, even ASCII characters cannot be exchanged unless the communications software being used makes appropriate conversions. Commodore computers are notable in this regard, using a nonstandard ASCII. With these, the problem is usually transparent to the user because the software required for the conversion is either built into or supplied with Commodore modems. The use of a standard modem, however, would require conversion software.

An additional problem is with control codes which may be incorporated into a file to be transferred. Another computer may use different codes for line feeds, carriage returns, cursor positioning, or printer control. This can give strange results when information is transferred between computers of different manufacturers or if different printers are used on the communicating systems.

As a result of the differences in graphics and control codes, many bulletin boards are machine specific. That is, even though text communication works well, programs cannot be uploaded to the host or downloaded and run on the user's computer. Unfortunately, the ability of computers to converse fluently is limited and probably will remain so as long as the technology is changing rapidly. Although software that allows one computer to emulate another exists for

a number of computers, it is expensive, limited in capability, and not readily available to most users. Even when available, a software package for each type of computer involved is required.

These comments are offered only for clarification because, overall, the author illustrated well the role of the microcomputer for both forensic science laboratory and personal use. Even one of the applications described can justify the acquisition of a microcomputer system, and the ability to simply and inexpensively add others makes a micro-based system a highly cost-effective productivity enhancement in the forensic science laboratory.

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Author's Response

Sir:

Charles Midkiff's comments to my article "Microcomputers in Forensic Science" bring up three important technical points that deserve a reply.

1. *Graphics*—There is a problem with modeming graphics (graphs, charts, pictures) directly between computers because of the variety of ways different computers assimilate graphic data; however, graphics are derived from raw data which can easily be sent over modem (for example, DIF files) and used by most computers to create the needed graphics using their own software routines. To make an analogy, different artists paint differently but if you give each a detailed enough description, you will get (slightly more or less) the same basic picture. In this case the modem can send the needed descriptions.

2. *Nonstandard American Standard Code for Information Interchange (ASCII)*—Most computer code sent over the phone lines is in standard ASCII code. Most computers can understand this code regardless of the brand or make. There are some inexpensive computers like the Commodore (\$100 to \$300) which have nonstandard ASCII code; however, there are inexpensive conversion programs and modems now available which will convert to standard ASCII. Because of the memory limitations of the Commodore, it is unlikely that anyone would be using this machine for serious telecommunication.

3. *Control codes*—Control codes are specialized signals that will direct the way data is received (for example, uppercase, line feeds, returns, and so forth). There are a great variety of these codes and they mean different things to different computers. A control code for a line feed (next space) in Brand A computer may signal a form feed (next sheet of paper) in another system. This problem can be handled by (a) using standard modem software parameters (for example, Source, Compuserve), (b) identifying which parameters you are using so the receiving computer can make the necessary option changes in its modem software, and (c) send a copy of your modem software to the receiving computer (over modem, of course).

Many of these problems can be handled by a call to your local computer dealer. If you are interested in more information on forensic science computers, I suggest you read my book *Computers for Professional Practice*, ISBN 0914555-00-6, Andent Press (available at your book store for \$15), or get copies of *Dental Computer Newsletter* and the *Journal of American Association of Forensic Dentists*.

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The Snowflake Paradigm

Sir:

The assumption of absolute uniqueness on the part of all tangible objects is a doctrine that has pervaded the interpretation of physical evidence. The doctrine generally takes one of two forms. The first is the metaphysical argument advanced by a number of classical philosophers (Heraclitus, Parmenides, Zeno, and Plato), and further developed in the 17th century by Leibniz [1]. This argument states that an object can be identical only to itself. The argument has been further extended [2] to the point where an object cannot be identical even to itself—the reasoning is that since an object is described by an infinite number of predicates, and since *time* is a legitimate predicate, an object is unique in a temporal sense as well. The metaphysical argument is generally accepted as true, but exists at a level of abstraction such that it is not of much utility in any practical application to the examination of physical evidence.

The second form of the uniqueness argument is the one invoked for forensic science purposes. It too is generally accepted as true, but since it has an empirical component it is probably not susceptible of direct testing. This form of argument is frequently voiced as "Nature never repeats itself," and is attributed to the Belgian statistician Quetelet. (As an aside, what Quetelet actually said [3] was that "Nature exhibits an infinite variety of forms." This would not address *processes* [for example, lightning striking in the same place twice]. However, this is quibbling.)

The empirical form of the uniqueness argument is applied to forensic science problems along the lines of the following: "No two snowflakes are alike, therefore no two . . . (gun barrels, fractured window panes, etc.) are alike." Whether the latter clause stems from the former is not the issue here. The issue is that the snowflake is frequently singled out as a paradigm of uniqueness. There is something about the paradigm that "has a nice ring to it." There is little doubt but that it has an intrinsic appeal to the lay public, from which of course juries are drawn.



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How do we know, or why do we believe, that snowflakes are unique? (Snowflakes can in fact assume an enormous variety of shapes—needles, prisms, plates, hollow prisms, bullet clusters, and so forth—depending on the history and career of the crystal as it grows in a cloud; for purposes of this discussion, however, a snowflake is taken to mean a planar dendrite—a flat crystal with delicate branches that is almost universally regarded as the archetypical snowflake.) Many observers, including Kepler in the 16th century [4], have noted the *highly individual* nature of snowflakes. Bentley [5] and Nakamura [6] have examined and photographed hundreds of snowflakes, all of which are clearly distinguishable from one another. But *hundreds* of snowflakes could fit in a lemur's fist. The caveman in the B.C. cartoon looked

at over 8×10^5 , but even this is a small number relative to the entire global production of snow for even a single year.

If the uniqueness of snowflakes (and, by extension, objects of evidentiary significance) cannot be established by direct observation, then perhaps another proof is possible. (The reason that this has not been done before is probably because everyone else has had better things to do.) The mass of snow formation is currently estimated at 24×10^{17} g per year [7]. Since the thermal characteristics of the earth have shifted over time, however, this value is applicable only since the end of the Juraissic age, about 130×10^6 years ago. (Undoubtedly there was snow somewhere on earth before that, but there no sentient beings to reflect upon its form.) If one assumes a yearly production of 24×10^{17} g of snow over 130×10^6 years, then 3.12×10^{26} would be a rational approximation of the number of grams of snow produced. Assuming that a typical snowflake weighs 10^{-5} g (a fledgling snowflake, with all its inherent intricacies, may weigh as little as 10^{-6} g while an elderly specimen may weigh 10^{-4} g [8]; a median value of 10^{-5} g is taken for these calculations), then approximately 3.12×10^{31} snowflakes have been produced over the past 130 million years. For those who wish to be reminded of scale, 10^{31} is approximately the number of millimetres that light would travel in 10 trillion light years.

That is a whole bunch of snowflakes. Couldn't there have been *one* coincidental replication in those 10^{31} snowflakes? Avogadro's Number (6.023×10^{23}) gives us the number of molecules per mole of snow, and from this we can calculate the number of molecules of ice in a 10^{-5} -g flake. The number is 3.35×10^{17} molecules. We cannot ask, however, whether it is possible to arrange 3.35×10^{17} molecules in so many different ways that no replication would be likely in 3.12×10^{31} snowflakes; the reason for this is that we cannot take molecules one at a time in determining possible arrangements. Ice crystallizes in 120° rhomboid units of two layers, each containing ten molecules [9]. Three unit cells form a hexagonal solid of sixty molecules, representing the simplest complete crystal of ice [10]. Then a typical snowflake has six sides or six branches; this represents a threefold symmetry (that is, a 120° replication), so we must divide first by 60 and then again by three, giving $2.16 \times 10^{15} \sim 10^{15}$ molecules. Could 10^{15} molecules be arranged so that replication is likely, or even remotely possible, in 10^{31} snowflakes?

It isn't likely. The number of possible arrangements of 10^{15} molecules is approximated by $n!$ in Sterling's Approximation [11]:

$$(2n\pi)^{1/2} (n/e)^n < n! < (2n\pi)^{1/2} (n/e)^n [1 + (1/12n - 1)]$$

(where $e = 2.718\ 28 \dots$).

Substituting 10^{15} for n and ignoring the trivial shrubbery in Sterling's formula (for example, $(10^{15}/2.718\ 28) \sim 10^{15}$), we arrive at the approximate figure of $10^{15(10^{15})}$ different arrangements. This number is virtually beyond human comprehension, and relegates the 10^{31} snowflakes to insignificance. Even then, we may not have fully developed the mathematics concerning the true uniqueness of a snowflake. Stirling's Approximation of $n!$ gives us the number of different *orderings* of n *distinguishable* ice units. In other words, what we have done here is to determine the number of ways that n distinguishable 60 molecule ice units could fit into any given single snowflake arrangement. Another approach to the uniqueness question, and one which would impart still greater complexity, would be to consider the geometrical *arrangements* of the 60 molecule ice units rather than the particular *ordering* of the units. The number of these arrangements would depend on the number of nonconstrained faces on the ice crystal where neighbors would be permitted to join. Our knowledge of the considerations applicable here are still sketchy [12], but there is every indication that the attendant considerations are incredibly complex and susceptible to subtle operative nuances.

On the basis of all of the foregoing, the present author is satisfied with the uniqueness of snowflakes. Unlike snowflakes, however, gun barrels are not made in clouds, and the proof of uniqueness of other objects must be based on yet other grounds.

Acknowledgment

The B.C. cartoon is reprinted with the permission of Jimmy Hart and Field Newspaper Syndicate.

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Relative Intensities of Selected Ions of Methaqualone-Related Isomers

Dear Sir:

The 16 mass spectra presented in the article by Dal Cason et al "Identification of Some Chemical Analogues and Positional Isomers of Methaqualone" (Vol. 26, No. 4, Oct. 1981, pp. 793-833) in the *journal* provided rich information concerning the fragmentation characteristic of methaqualone-related positional isomers. It appears that a clearer and less complicated correlation between the intensities of properly selected ions and the position of substitution groups can be established.

We have measured and calculated the relative intensities of characteristic ions, m/z $[M - R]^+$, $[M - CH_3]^+$, M^+ , $[R + 76]^+$, and $143 [I]$ ($R = CH_3$, F, Cl, Br, or I) from the line diagrams provided in the original article and presented these data in Table 1. While the detailed fragmentation pathways cannot be readily deduced from these spectra alone, the relative intensities of these ions show explicit correlation with the position of halogens in these compounds (Fig. 1). With respect to $[M - R]^+$ ($R = F$, Cl, Br, or I) ion, the formation of the other ions listed in Table 1 are favored in the following order: *ortho* < *meta* < *para*. In the case of tolyl derivatives, this correlation is complicated by the presence of the second methyl group.

Compared to the multiple sets of ion cluster intensity ratios (Table 4 of the original article)

TABLE 1—Structure and EI MS characteristics of methaqualone congeners.^a

Compound Name	R ₁	R ₂	R ₃	Mol. Wt.	% ^b of [M - R] ⁺	Int. Ratios ^b [M - R] ⁺ : [M - 15] ⁺ : M ⁺ : [R + 76] ⁺ : 143
2-Methyl-3-phenyl-4-Q ^c	H	H	H	236	72	
2-Methyl-3- <i>o</i> -tolyl-4(3H)-Q	CH ₃	H	H	250	100	1: 1 ^d : 0.86 : 1.0 : 0.33
2-Methyl-3- <i>m</i> -tolyl-4(3H)-Q	H	CH ₃	H	250	93	1: 1 ^d : 0.70 : 1.1 : 0.030
2-Methyl-3- <i>p</i> -tolyl-4(3H)-Q	H	H	CH ₃	250	81	1: 1 ^d : 0.96 : 1.2 : 0.97
2-Methyl-3- <i>o</i> -fluorophenyl-4-Q	F	H	H	254	100	1: 0.76 : 0.90 : 0.56 : 0.54
2-Methyl-3- <i>m</i> -fluorophenyl-4-Q	H	F	H	254	21	1: 3.9 : 4.5 : 4.5 : 2.5
2-Methyl-3- <i>p</i> -fluorophenyl-4-Q	H	H	F	254	8.3	1: 8.8 : 11 : 11 : 7.2
2-Methyl-3- <i>o</i> -chlorophenyl-4-Q	Cl	H	H	270	100	1: 0.29 : 0.19 : 0.88 : 0.33
2-Methyl-3- <i>m</i> -chlorophenyl-4-Q	H	Cl	H	270	57	1: 1.2 : 1.6 : 1.8 : 1.1
2-Methyl-3- <i>p</i> -chlorophenyl-4-Q	H	H	Cl	270	38	1: 2.0 : 2.6 : 2.7 : 2.3
2-Methyl-3- <i>o</i> -bromophenyl-4-Q	Br	H	H	315	100	1: 0.050 : 0.056 : 0.25 : 0.083
2-Methyl-3- <i>m</i> -bromophenyl-4-Q	H	Br	H	315	86	1: 0.17 : 0.29 : 0.33 : 0.53
2-Methyl-3- <i>p</i> -bromophenyl-4-Q	H	H	Br	315	25	1: 0.96 : 1.8 : 1.3 : 3.0
2-Methyl-3- <i>o</i> -iodophenyl-4-Q	I	H	H	362	100	1: 0.047 : 0.11 : 0.36 : 0.13
2-Methyl-3- <i>m</i> -iodophenyl-4-Q	H	I	H	362	43	1: 0.56 : 1.3 : 0.58 : 0.77
2-Methyl-3- <i>p</i> -iodophenyl-4-Q	H	H	I	362	19	1: 1.4 : 3.1 : 1.1 : 4.0

^aSee Fig. 1 for the positions of R₁, R₂, and R₃ groups, the *m/z* [R + 76]⁺ and 143 ions.
^bIntensities of these ions are measured (with a ruler) from the line diagram of the mass spectra provided by the original article. Their relative intensities are then calculated. R represents CH₃, F, Cl, Br, or I.
^cQ: quinazolinone.
^dIn tolyl derivatives, intensity correlations of the [M - R]⁺ ion to the other ions cannot be readily established because of the presence of two methyl groups in the same molecule, both contributing to the formation of the [M - R]⁺ ion.

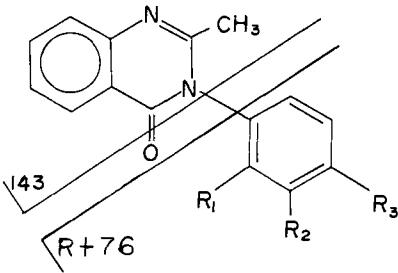


FIG. 1—Structural framework of substituted quinazolinones. (See Table 1 for the names and substitution groups of individual compounds.)

used in the authors' analysis, the distinct pattern described here provides a simpler, yet more effective approach for the differentiation of these positional isomers.

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