Diverse fingerprints

The article "Fingerprinting the unusual suspects" by David Bradley (December 2003, p 33) commented on the technique of affinity fingerprinting (e.g., Beroza, P.; et al. *Drug Discov. Today* **2002,** *7,* 807–814) in the context of virtual and high-throughput screening. This methodology captures experimentally determined binding profiles of small molecules to selected proteins and uses the resulting affinity patterns as a predictive tool for compound selection. Figure 1 of this article was adapted from a previous publication (Bajorath, J. *J. Chem. Inf. Comput. Sci.* **2001,** *41,* 233–245; Figure 4). This figure summarizes the results of various similarity search calculations on peptidomimetics.

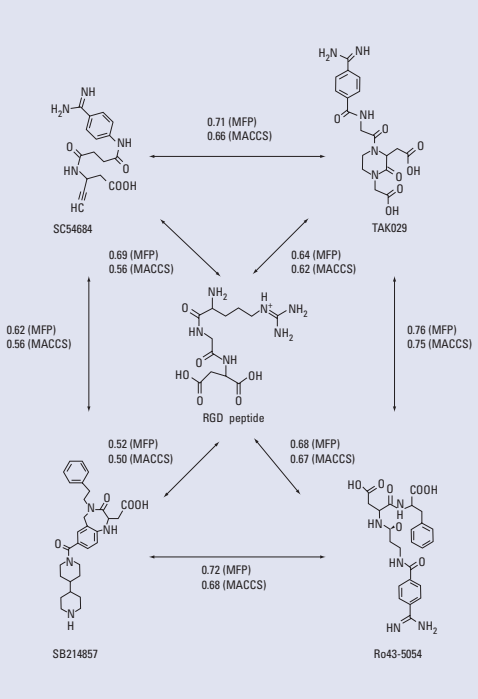

Figure 1

However, in contrast to what was stated in the article, these results were obtained not by using affinity fingerprints but by using molecular fingerprints consisting of structural fragments and other two-dimensional molecular descriptors. Furthermore, in the caption of Figure 1, the use of these fingerprints is described as pharmacophore fingerprinting. Pharmacophore fingerprints are designed to monitor all possible spatial arrangements of a defined multiple-point pharmacophore in a molecule (and are thus three-dimensional in nature). In contrast, the two-dimensional fingerprints used to produce the results shown in Figure 1 do not contain explicit pharmacophore information and are distinct in their design.

For a review of different types of fingerprints and similarity search tools, see, for example, Bajorath, J. *Nat. Rev. Drug Discov.* **2002,** *1,* 882–884.

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Editors' reply:
We regret that the caption in Figure 1, which we adapted from your 2001 *JCISC* paper, did not accurately represent the information that David Bradley presented about your work in the article he wrote for us. The incorrect choice of figures to illustrate Bradley's article was our error.

Terminate the term?

Why do we use archaic terminology ("Fingerprinting the unusual suspects") when describing new biologic techniques such as DNA, affinity, and other new-technology printing when a more up-to-date terminology should be used? When the jet plane was invented, it was not called the "jet propeller plane", because there was no propeller involved. The same applies to the new biologic printing techniques; there is no finger involved. Why not use a term that fits, which would be the "bioprint"? We need to modernize our terminology and get out of the 18th century. Maybe someone else can think of a better term than bioprint, but it is time to put the old term "fingerprint" to rest.

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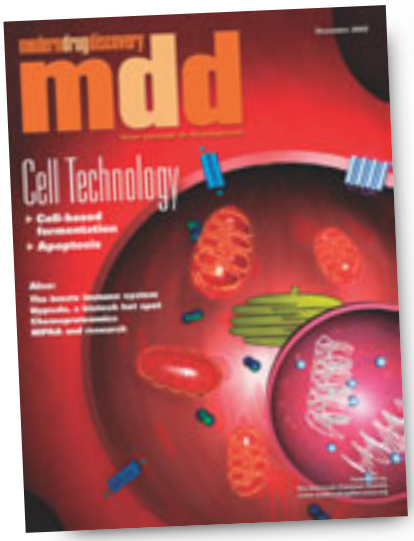

Give nature its due

In the News in Brief article "Natural products aMASSed" (December 2003, p 16), Randall Willis's introductory sentence stating that natural product research is largely untapped for therapeutic agents makes me fidget. Natural product research *is* the area that brought us the earliest therapeutic agents, from salicylic acid to penicillin to yohimbine alkaloids to, most recently, Taxol. Some appreciation of this would have sufficed.

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Author's reply:
My statement was actually made as something of a complaint. In this era of high-throughput technologies, I believe that a lot of drug discovery scientists are missing a great opportunity to identify novel compounds rather than simply make a new variation on something that sits in a chemical library. With this in mind, I wrote "Nature's pharma sea" (*MDD,* January 2002, p 32), which describes some of the then-recent efforts by pharmaceutical firms to identify and characterize new druglike compounds from marine sources.

Randall C. Willis