one of them will be better for search from the library. Thus, for example for the two close vectors (1,2,3,4,5) and (1,2,1,3,4,5) $\cos\theta$ is 0.999916 while Pearson's r is equal to 0.999643. To see it more clearly we should look on their deviation from unity, which is the criterion for dissimilarity. In the case of $\cos\theta$ it is $8.4 \cdot 10^{-5}$ while for r it is $3.57 \cdot 10^{-4}$. Another example is (1,2,3,1,4,1,5) and (1,2,1,3,4,5,2) where $\cos\theta$ is 0.999426 and Pearson's r is 0.99694, i.e. the dissimilarities are $5.74 \cdot 10^{-4}$ and $3.06 \cdot 10^{-3}$.

Another advantage of r on any arbitrarily defined similarity index is that its calculation is already one of the function of several spread sheets as for example in Excel it is the either the CORREL or PEARSON functions. These two functions are actually the same function, written by different but equal equations.

We perform similar tests for identification in order to identify the location of a radioactive point source in the lung using four gammas detectors [6] and comparing the 4-dimension vector of counts of supposedly unknown source with the appropriate vectors of 56 standard points. It was found that for 224 "unknown" measurements the $\cos\theta$ test hit correctly 182 cases (81.3%) while Pearson's r hit the correct answer only in 159 cases (71.07%). Thus while r is more sensitive to small changes in the vector components, $\cos\theta$ is a better test for identification.

REPLY

¹We wish to reply briefly to the criticisms made by Dr. Alfassi in the accompanying article. Dr. Alfassi ignored the intention of our Application Note. Our purpose was to provide and evaluate methods for comparing product-ion spectra obtained by MS/MS in ion-chemistry or structure studies. The goal was a strategy that could be easily implemented using standard programs (e.g., Excel) by an individual investigator who is occasionally faced with the requirement to compare spectra of an unknown and a reference. In the article, we described a modification of the similarity index (SI), which we had published some years ago (Reference 5 in the Alfassi article), and compared it to an established method (spectral contrast angle), using both real and simulated data. For these instances, there is no library of spectra available, unlike for EI spectra, and the requirement for the investigator to modify a library-search algorithm is too onerous. Furthermore, Stein and Scott [1] already compared these two approaches, and three others, in a library-search evaluation and found that the spectral contrast angle is superior. Thus, the criticism that we failed to test the two approaches by using a library of spectra misses the point.

Another criticism is the "artificiality" of the comparison of the two methods. This criticism can be leveled at most comparison schemes. Clearly one can amplify the differ-

An important advantage of the $\cos\theta$ test on the Euclidean distance test [2] is that it does not require normalization. If correct normalization is done (i.e. normalizing the vectors to have unit length) than $\cos\theta$ and the distance are equal tests since $d^2 = 2(1 - \cos\theta)$. Stein and Scott [2] obtained different results for the $\cos\theta$ and Euclidean distance tests because they normalized differently their vectors.

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ences in any comparison by a mathematical operation. Dr. Alfassi chose to take the cosine of the angle of the spectral contrast angle and diminish its ability to distinguish. We could have chosen to enhance it by raising it to some arbitrary power. Nevertheless, our test for effectiveness was a statistical evaluation, which was not done by Stein and Scott [1]. We showed that our data sets could be distinguished in a statistically significant way with one method (i.e., spectral contrast angle) and not the other.

Furthermore, the comparison was of ratios where each value was divided by the self-value, allowing us to compare dimensionless numbers. Thus, we do not understand Dr. Alfassi's comment that the "basic error is that we are comparing criteria with different dimensions."

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