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Discussion

Reply to ‘‘Comments on predictive strategies for determining retention indices’’

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In the preceding paper, Peng [1] has highlighted a few points in a publication of ours [2], that he considers to be misleading. We would like to thank him for the analysis and to make a few comments on these.

When we normalized the *A* values in our Eqs. 5a and 6a to 100, the new group retention factors (GRF values) obtained for the allylic alcohol moiety (726 for the polar column and 144 for the non-polar column) left the situation pretty much unchanged for the allylic alcohols on the respective columns (Tables 2 and 3). In Tables 4 and 5, however, when applied to nerol and geraniol, these new values resulted in improved percentage differences between I_{obs} and I_p for the polar column (-0.99 and -0.98, respectively). On the non-polar column the percentage differences went to -5.7% in each case, which was closer to Peng's data. The chromatographic system we used was originally assessed and found to compare very closely with that of Peng and his group.

In his second point, Peng questioned our calculations for nerol, geraniol and linalool. He said that we included in our calculations, GRF values for the tertiary carbon and *cis–trans* configuration for linalool, and for no apparent reason left them out in the cases of nerol and geraniol. He further stated that had the GRF contributions for tertiary and quaternary carbons and *cis–trans* configuration in these molecules been included, as they should be, then the percentage difference between I_{obs}, I_p and I_{cp} values would have been considerably smaller than those shown in Tables 4 and 5. In the case of linalool, we included in our calculations a GRF contribution for the tertiary carbon. We did not apply a GRF contribution for *cis–trans* isomerism, as no such isomerism exists in this molecule. For nerol [(*Z*)-3,7,-dimethyl-2,6-octadien-1-ol] and geraniol [(*E*)-3,7-dimethyl-2,6-octadien-1-ol], no tertiary or quaternary carbon atoms are present in these molecules, thus no GRF for either of these was applied. Please note, however, that in Tables 3 and 4 of our publication [2], the values for the tertiary carbon on the polar (-75 i.u.) and non-polar (-50 i.u.) columns were regrettably omitted from the definitions preceding the data. These values were however included in our calculations for linalool on both columns, and this could have been misleading.

In relation to Peng's comments on predicting the retention behavior of esters, the definitions stated by him for ΔI and GRF must be accepted in principle. In conclusion, we studied the homologous series of

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geranyl and linalyl esters to gain a better understanding of the various interactions occurring in these molecules, and proposed some ideas on the factors which could influence retention in these polyfunctional systems [2].

References

[1] C.T. Peng, J. Chromatogr. A 808 (1998) 277–278.
[2] G.I.C. Simpson, Y.A. Jackson, J. Chromatogr. A 766 (1997) 141–146.