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Discussion

# Reply to ''Reply to ''Comments on predictive strategies for determining retention indices''''

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In the third paragraph of their ''Reply'' paper [1], Simpson and Jackson stated that, ''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 factor for either of these was applied''. Nerol and geraniol are *cis–trans* isomers of the terpene alcohol, 3,7-dimethyl-2,6-octadien-1-ol. The carbon atoms 3 and 7 in the molecule are each connected by two single bonds and one double bond to other carbon atoms and are thus considered by convention to be quaternary or tertiary carbon atoms in nature. The difference between the carbon atoms in a molecule can be detected by $^{13}$C NMR spectrometry. Since these carbon atoms are not normal alkane carbon atoms, the algorithm for retention index prediction also requires that they be assigned a GRF value.

Linalool (3,7-dimethyl-1,6-octadien-3-ol) is also a terpene alcohol but differs from nerol and geraniol in having the hydroxyl group on carbon atom 3 instead of 1 and the double bond at carbon atom 1 instead of at 2. Unlike nerol and geraniol, linalool is a tertiary alcohol. How to partition the GRF value of the linalool molecule between a hydroxyl group and a tertiary carbon atom is uncertain in this situation because the number of model compounds studied is very limited. This exemplifies the pitfalls and dilemma of retention index prediction in compounds with multi-functionalities.

## References

[1] G.I.C. Simpson, Y.A. Jackson, J. Chromatogr. A 808 (1998) 279–280.


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