

Supplementary information – additional figures

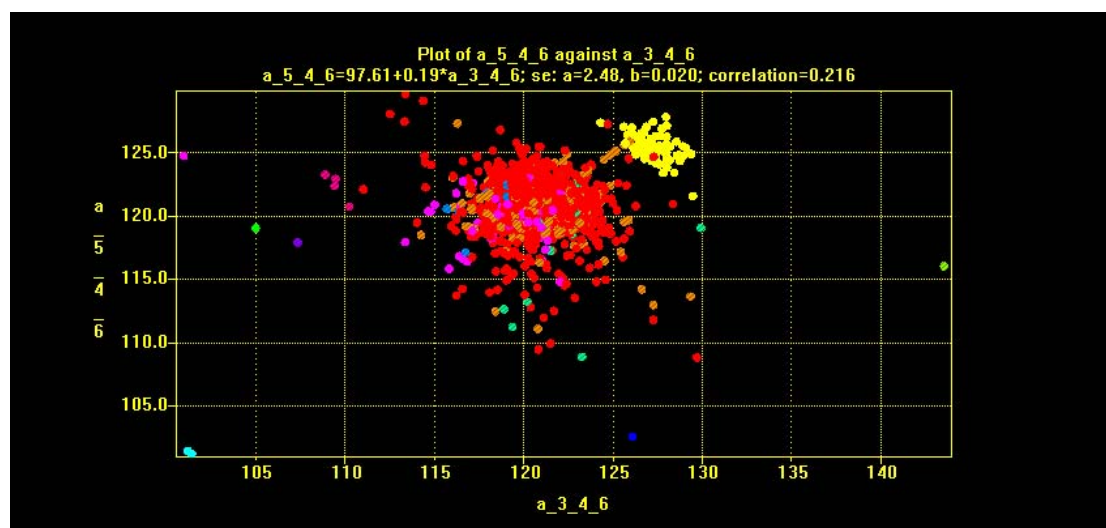


Figure 1 Scatterplot of the C(5)-C(4)-O(6) angle against the C(3)-C(4)-C(6) angle. Sample colours are as in Figure 2.

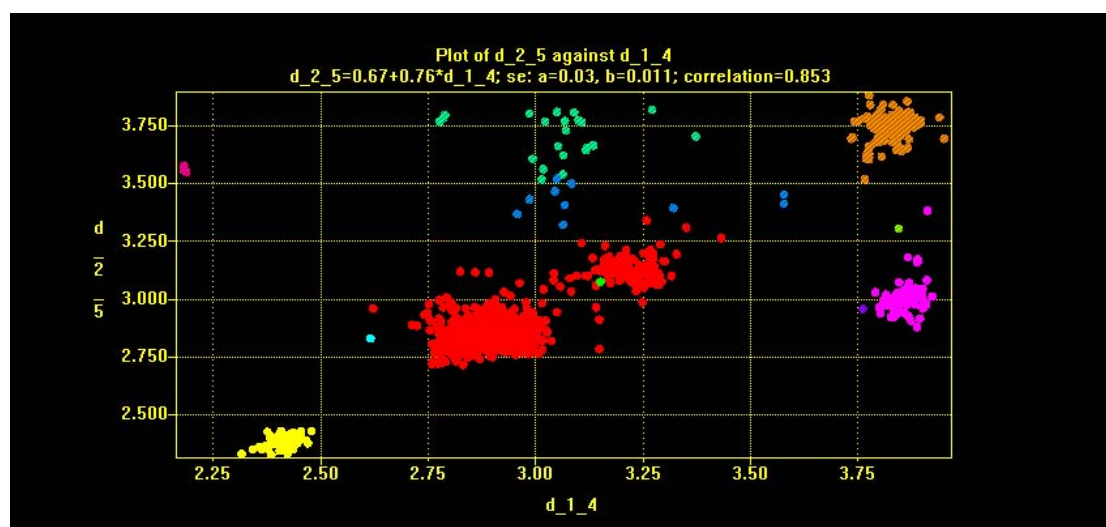


Figure 2 Scatterplots of the C(2)-C(5) distance against the C(1)-C(4) distance. Sample colours are as in the dendrogram (Figure 2 in main document)

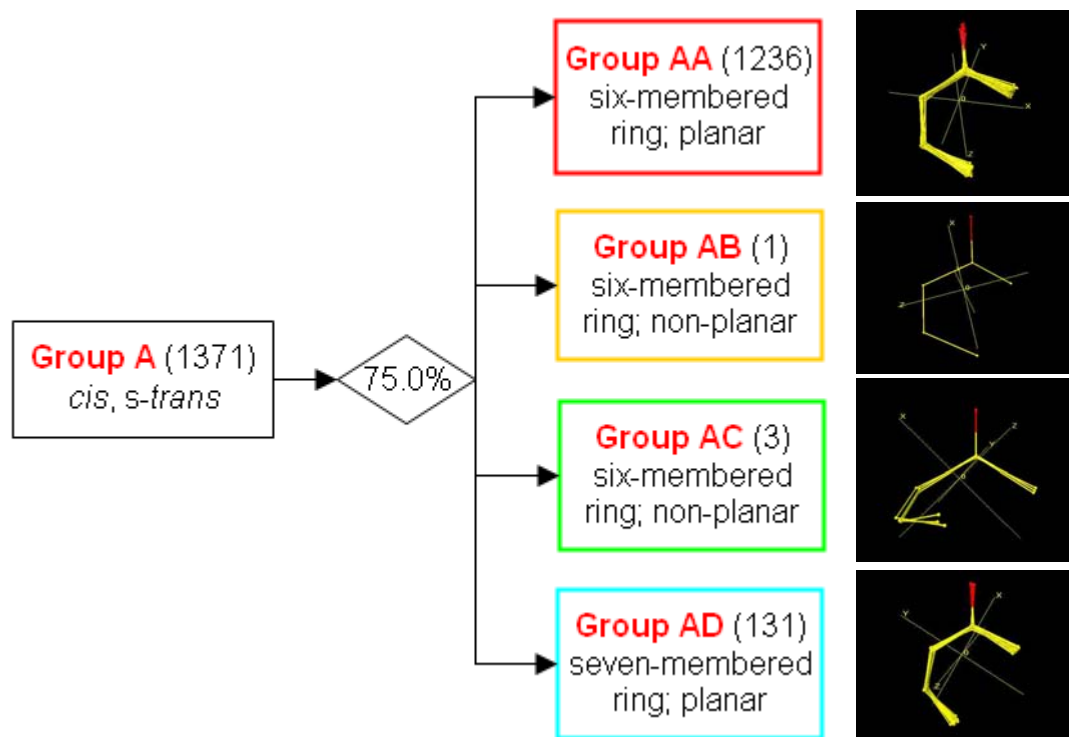


Figure 3 Decision tree of enone geometries for the re-clustering Group A (see Figure 5).

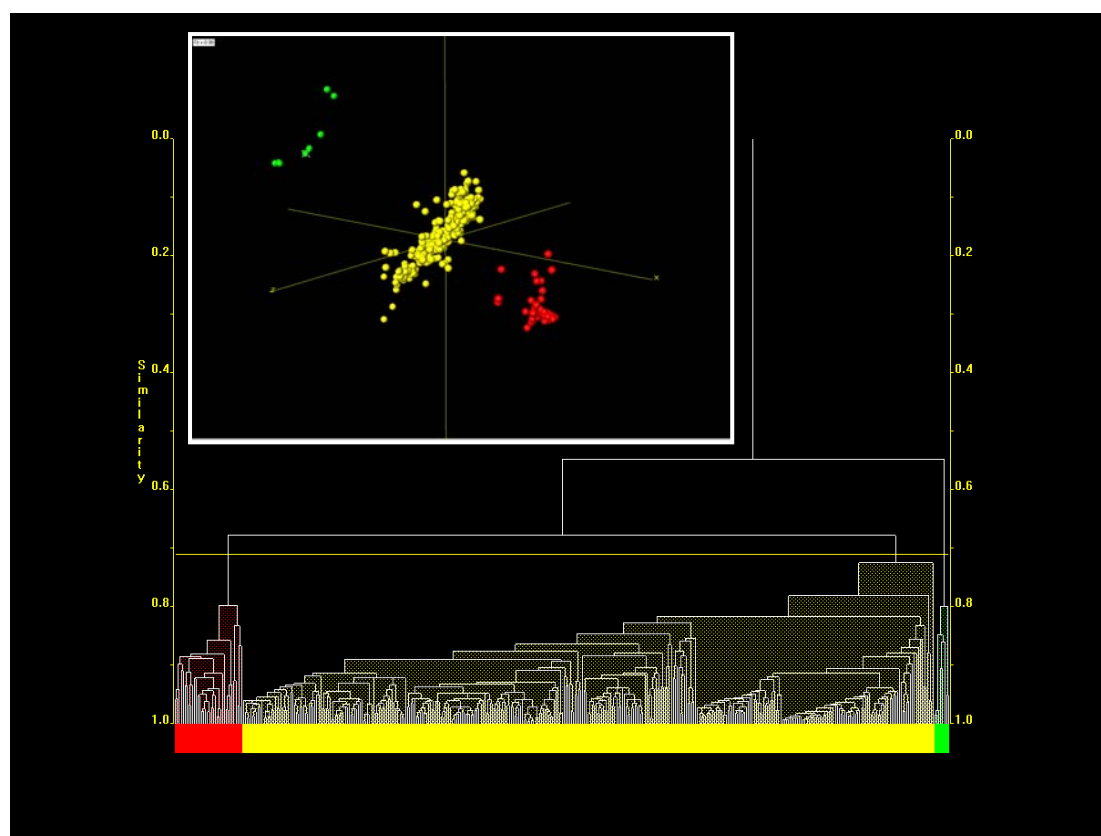


Figure 4 Dendrogram and MMDS plot (inset) for re-clustering enimine Group A.

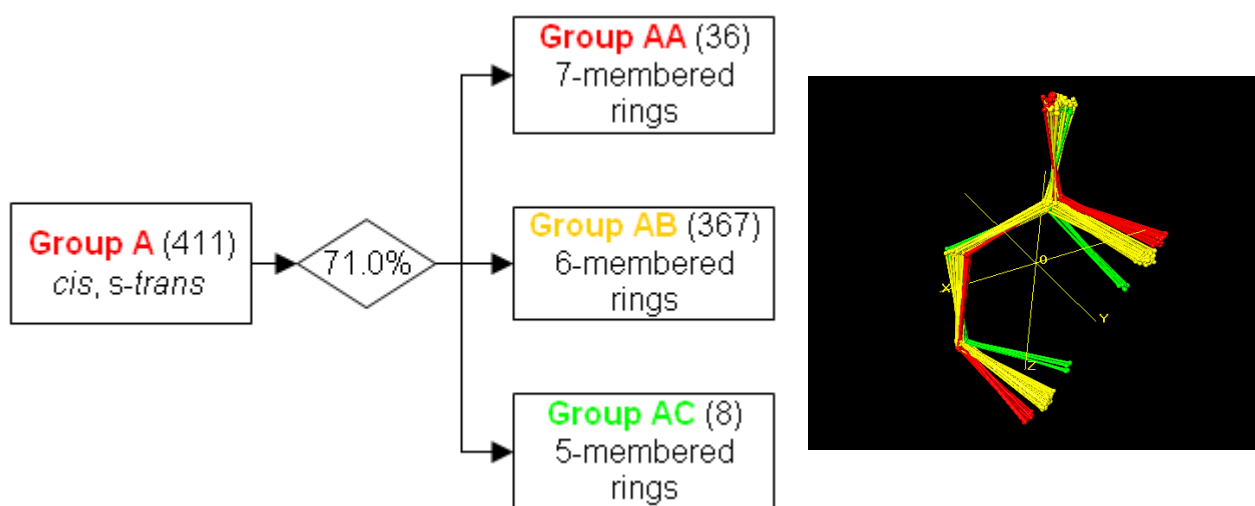


Figure 5 Decision tree for distribution of geometries for re-clustering Group A.

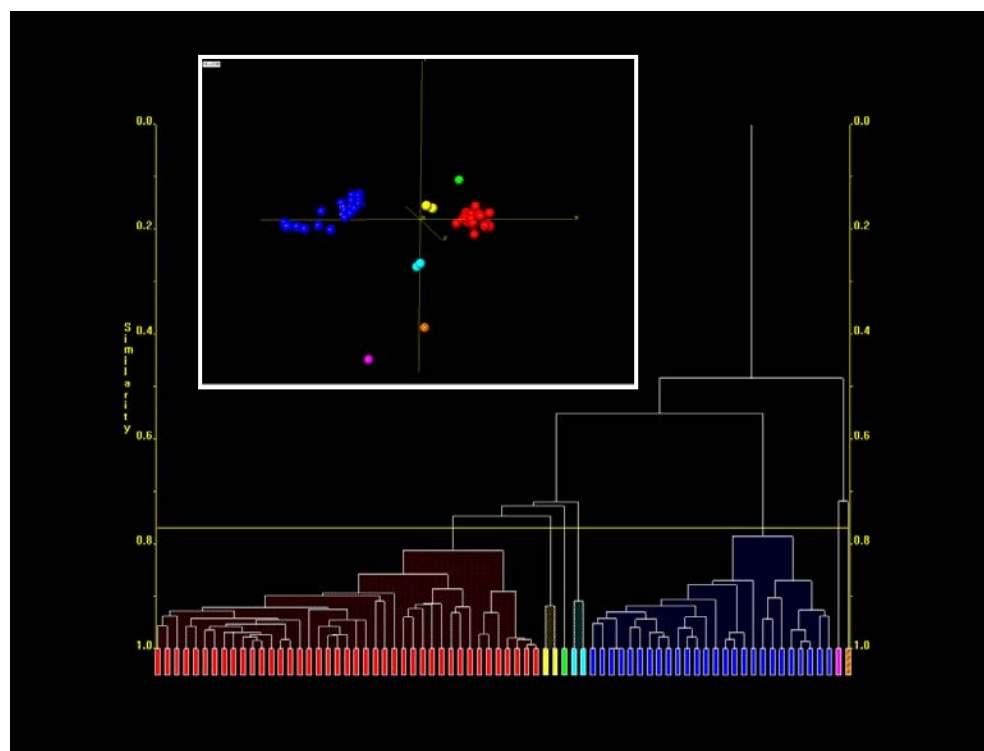


Figure 6 Dendrogram and MMDS plot (inset) for re-clustering enamine Group E.

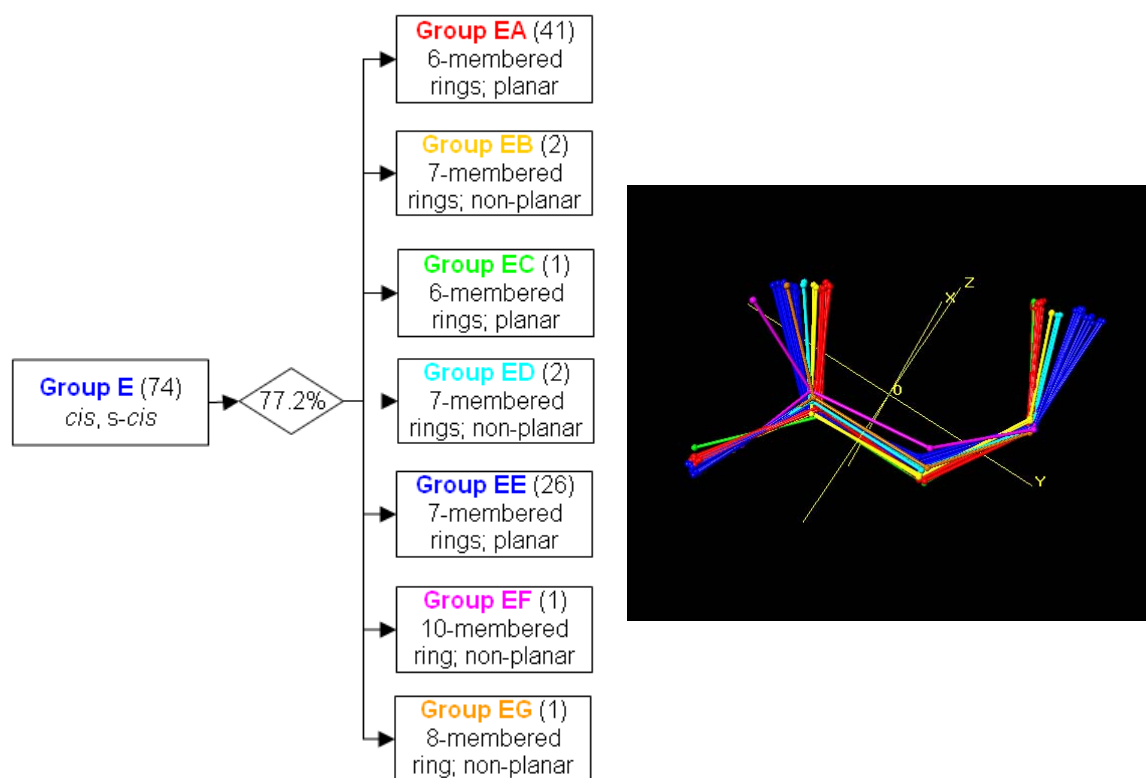


Figure 7 Decision tree for distribution of geometries for re-clustering Group E, with overlay of the fragments.

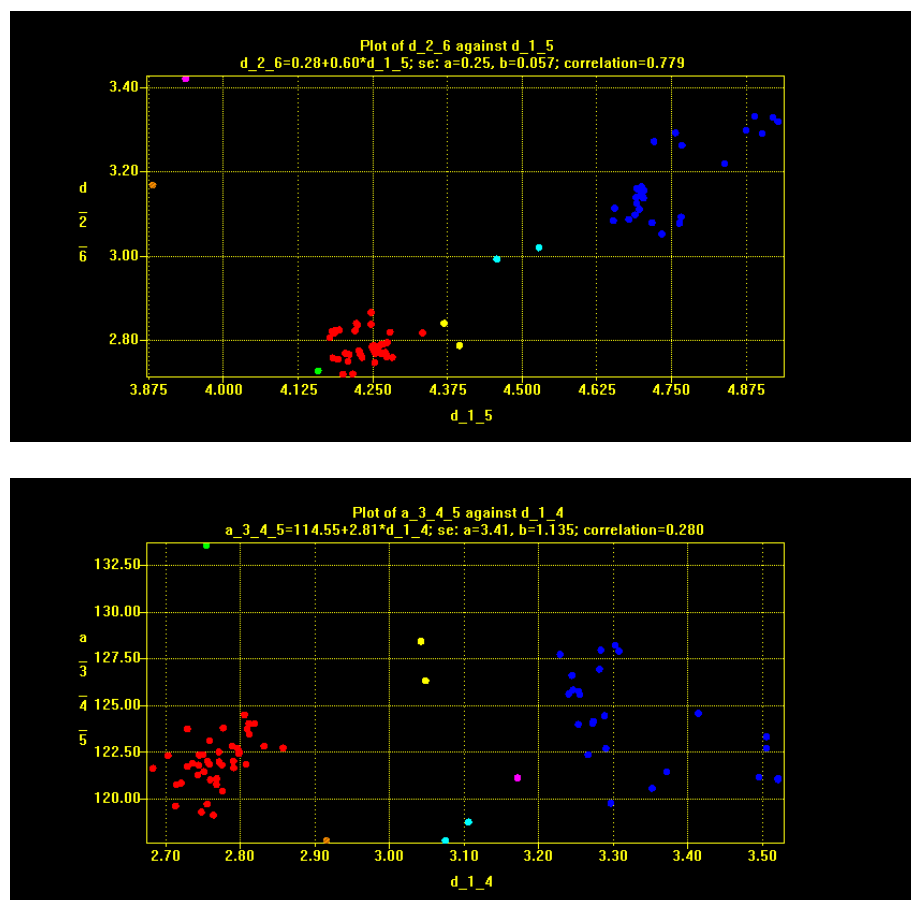


Figure 8 Scatterplots of the C(2)-N(6) distance against C(1)-C(5) distance (top) and C(3)-C(4)-C(5) angle against C(1)-C(4) angle (bottom).