

Procrustes analysis as an aid for aligning molecules in medicinal chemistry

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Abstract

A common problem in medicinal chemistry is that the spatial arrangement of the atoms in similar molecules is known, but that it is difficult to sort out to what extent these molecules are the same and to what extent they are different.

Within the social and behavioural sciences, and also food sciences, Generalised Procrustes Analysis (Gower, 1975) is often used to align configurations from different analyses to assess them with respect to each other. Commandeur (1991) in his thesis developed a variant of generalised Procrustes analysis which could handle different numbers of rows in different samples. It especially this feature which makes it possible to use the technique for aligning molecules, which have both common and unique atoms. Some or all of the common atoms can be used as "backbone" for the Procrustes analysis. By aligning the backbone, automatically the arrangements of the other atoms of the molecules can be assessed with respect to other. By using publicly available software, visual representations can be made of the aligned molecules, so that their differences stand out.

References

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