Assignment of the Absolute Configuration by ^{1}H-NMR: From Mono to Polyfunctional Compounds

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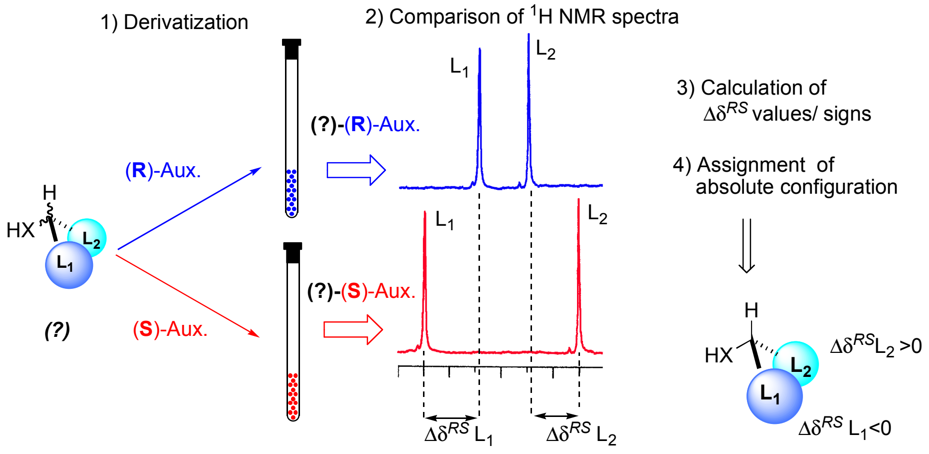
The assignment of the absolute configuration of organic compounds by NMR is particularly useful when no monocrystals are available and a rapid and inexpensive method is needed. In its classical approach, the substrate is separately derivatized with the two enantiomers of a chiral auxiliary reagent and the absolute configuration is obtained by comparison of the H-NMR spectra of the two resulting diastereomers (1). In this presentation I will show first, the foundations of this procedure: the role of the anisotropic group of the auxiliary and the importance of the conformation. Next, the use of the auxiliary reagents (arylmethoxyacetic acids: MPA, MTPA, and 9-AMA; the protected aminoacid BOC-PheGly and the alcohol 9-AHA) for the assignment of the absolute configuration of chiral secondary and primary alcohols, primary amines and carboxylic acids, will be described.



Alternative procedures allowing the use of only one derivative instead of two or the suppression of any manipulation of the sample, will come next. Finally, the rules for assignment of the absolute configuration of polyfunctional compounds such as 1,n-diols, and 1,2,3-triols, will be presented (2).

REFERENCES:
1) Seco, J. M.; Quiñoá E.; Riguera R.; *Chem. Rev.* 2004, 104, 17-117
2) Freire, F.; Seco, J. M.; Quiñoá, E.; Riguera, R.; *J. Org. Chem.* 2005, 70, 3778- 3790. IBID *Chemistry Eur. Journal* 2005; IBID, *Org. Letters* 2005