

Obtaining information from the NMR spectra of complex mixtures: Pseudoseparation and classification by fingerprint

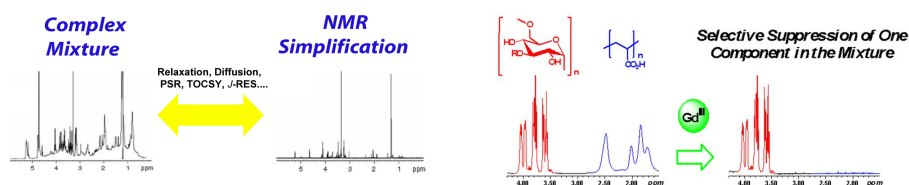
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The different methods to extract information from the NMR of complex mixtures (industrial, foods, beverages, biological fluids), without previous separation are described. In particular, procedures for selective pseudoseparations by electronic filtering based on relaxation, diffusion or coupling and by the use of selective paramagnetic spin relaxation ions or by combination of those techniques will be presented. Finally, the use of specific mathematical treatment of the data (NMR, MS, GC etc), for the automatic classification of complex mixtures (metabolomic approaches) will be presented and illustrated with examples in the food and medical fields.



References

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