Remarks on the Quality of ^{13}C-NMR Data published in the Chemical Literature

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Our NMR-data published today might serve as reference material for future investigations, therefore we have the responsibility to publish highly validated data. Different journals and authors seem to have a quite different understanding of the term 'validated data', as has been shown by correlating the quality of published NMR-data with the Impactfactor of the journal [1], furthermore the applied 'peer-reviewing' process seems to be outdated. From these arguments given here the pronounced need for automatic data validation – or at least consistency checks with already known facts – can be deduced. In a recently published, very comprehensive review [2] a workflow has been presented in order to avoid most of the common errors in signal assignment and structure elucidation of organic compounds.

A detailed analysis of the most frequent errors in CNMR-data of compounds taken from the field of natural product chemistry will be given. This analysis will start with trivial assignment errors, continued by obviously wrong structure proposals, followed by deducing different structure proposals from identical spectral data and culminate in the fully automatic revision of published natural products.

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[1] Robien W., Trends in Analytical Chemistry 28, 914-922 (2009)

[2] Robien W., Progress in the Chemistry of Organic Natural Products in A Critical Evaluation of the Quality of Published ^{13}C NMR Data in Natural Product Chemistry (Eds: A. Douglas Kinghorn, Heinz Falk, Simon Gibbons, Jun'ichi Kobayashi), Springer, Germany, **2017**, 137–215. ISBN: 9783319497129