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1D NMR Spectra do not work in QSPR

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About two years ago a student started with me to work on the use of 1D NMR and IR spectra in quantitative structure-activity relationship (QSAR) work, with the goal to show that these spectra contain 3D information relevent to QSAR models. It is known that these spectra depend on the 3D conformation of the molecule.

Half a year later we concluded that from the data which we started with (48 compounds with binding affinity), no conclusions could be drawn what so ever: no statistically sound models could be build at all. So, we composed three larger data sets. These sets, all QSPR data sets, did give us models, but all the spectra based models were worse than a Dragon descriptor based model using the same number of variables, without doing any variable selection.

I presented this work at the 7th ICCS in Noordwijkerhout half a year ago, and now got published in the JCIM: DOI 10.1021/ci050282s. Comments on this article are ***most*** welcome!