# Analytical Model for the Prediction of NMR Methyl-side Chain Order Parameters in Proteins

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## 1 Introduction.

An analytical model is presented for the prediction of NMR order parameters of methyl groups in proteins. The model, which is an extension of the local contact model for backbone order parameter prediction, uses a static 3D protein structure as input. It expresses the methyl-group S2 order parameters as a function of local contacts of the methyl carbon with respect to the neighboring atoms in combination with a term that takes into account the number of consecutive mobile dihedral angles between the methyl group and the protein backbone. For six out of seven proteins the prediction results are good when compared with experimentally determined methyl-group S2 values with an average correlation coefficient r=0.65±0.14. For cytochrome c2, which is an unusually rigid protein, no correlation between prediction and experiment is found. Despite its simplicity, it represents a first comprehensive relationship between protein NMR side-chain dynamics and protein structure.

## 2 Figures and tables.

The analytical model reads: $S_i^2 = \tanh\left(a \cdot C_i / n^b\right) - c$, where $a$, $b$, $c$ are empirical parameters, $C_i$ is the local contact experienced by methyl carbon $i$, and $n_i$ is the number of mobile covalent bonds between the methyl carbon $i$ and the backbone.

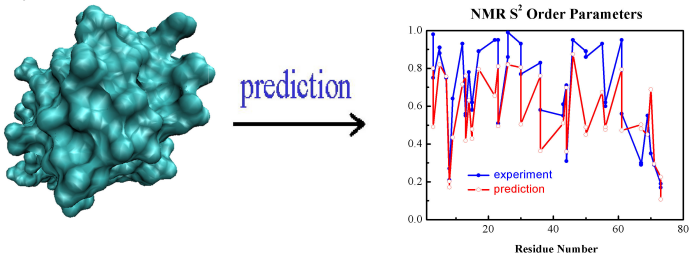


Figure 1: Prediction of ubiquitin methyl group order parameters using analytical model

## References

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