# A Structure Validation Concept Beyond the Static Resolution in Polymers

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Novel unorthodox approaches employing deep learning techniques can nowadays predict protein’s 3D structure owing to extensive training based on plausible x-ray structural data. However, native state of a biochemically active polymer is rather structure-dynamical. A validation of 3D polymer’s motives beyond static snapshots due to x-ray is obviously desirable. Their proper description within a training data set might enhance applicability of novel structure-predicting tools. Molecular dynamic simulation can extend structural picture of biopolymers towards structure-dynamic one; however, its accuracy is often questioned due to deficiencies of available force fields. Hence, only molecular dynamics validated against adequate *in liquid* experiment can illuminate true state of a biopolymer. We will introduce newly developed theoretical method for structure-dynamic interpretation of NMR spectra in polymers where a model of static 3D molecular structure is replaced by probability distribution for NMR-assigned geometrical parameter(s). So far omitted dynamical component in a training data could be resolved in this way.